

MATHEMATICS EXTENDED ESSAY

Fourier Transforms in Hybridization Theory

To what extent, can Fourier transforms model
the hybridization of an element?

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Table of Contents

1.0) Introduction.....	3
1.1) Rationale	3
1.2) Research Question	4
1.3) Structure of the Investigation	4
2.0) Background Information.....	4
2.1) Math.....	4
2.1.1) The Maclaurian Series	4
2.1.2) The $e^{\pi i}$ Transform and the Complex plane.....	10
2.1.3) Fourier Transforms	12
2.2) Physics and Chemistry Concepts required for the understanding of this investigation	12
2.2.1)The energy of an electron in an orbital'.....	16
2.2.2) Infrared Spectroscopy- the energy of a bond.....	18
2.2.3) Plank's Equation	18
2.2.4) Hybridization Theory.....	19
3.0) Using Math to develop the model'.....	21
4.0) Application of the Model.....	32
4.1) Analysis	37
4.2) Assumptions.....	37
4.3) Strengths	37
4.4) Weaknesses and Improvements.....	38
4.5) Implications.....	39
5.0) Conclusion	39
6.0) Extensions and Other Applications	39
8.0) Bibliography	41

1.0) Introduction

In 1822, Joseph Fourier invented the Fourier Series, with which any function could be approximated as a sum of waves. This technique, - the Fourier Series- was used to approximate multiple more complicated equations as a sum of easy-to-deal-with sine waves. The Fourier Series has applications in multiple areas of math.

Later, the Fourier transform was developed, in which waves were able to be expressed as a sum of others or broken into their constituents. This had multiple applications in the sciences.

1.1) Rationale

As an avid reader of physics, I found the concept of the Fourier transform in multiple research papers, and found that it could achieve almost magical things. This concept really did intrigue me and forced me to learn about it.

As a player of the guitar, I knew that I would be able to apply this math to my instrument, but on research, found that this had been done multiple times, and I could not bring myself to explore what was already explored. Instead, the concept of mixing appeared in a different part of the IB syllabus- Chemistry HL, Hybridization theory. Using my knowledge of Physics, Chemistry and Math, I developed my own theory, in how I could use Fourier transforms to mirror the process of Hybridization in atoms.

This approach was relevant to me, as Hybridization is my favourite topic in the IB, and exploring it was just about the only thing I could do as my EE. The theory of hybridization is supported by complicated models like the Schrödinger equation, but my theory would be simpler and easier to understand.

1.2) Research Question

The mentioned interest and understanding led me to the development of the following RQ.

To what extent can Fourier Transforms be used to predict the hybridization of an element?

1.3) Structure of the Investigation

The investigation will follow the following structure

- Mathematical concepts used will be explained.
- Necessary Physics and chemistry concepts will be explored.
- The approach to the Fourier transform will be explained, with an example.
- Fourier transforms will be applied to hybridization
- A conclusion and analysis

2.0) Background Information

2.1) Math

2.1.1) The Maclaurian Series

The Maclaurian Series is a form of approximation, where one can approximate any function as a polynomial around the point 0.

This can be done by matching coefficients of a polynomial to the function.

One can obtain information about the function through calculus. The first piece of information one can obtain is the value at 0. One can also match the derivative and the concavity and all information gained by taking successive derivatives.

Here is how one would do this for an arbitrary function¹

$$\text{let } F(x) = e^x$$

$$P(x) = C_0 + C_1x + C_2x^2 + C_3x^3 + C_4x^4$$

We can match the first few terms and later consider more.

First, one can match the y intercepts,

$$F(0) = 1$$

$$P(0) = C_0$$

Therefore $C_0 = 1$

One can observe how the polynomial looks, when it consists of only 1 term.

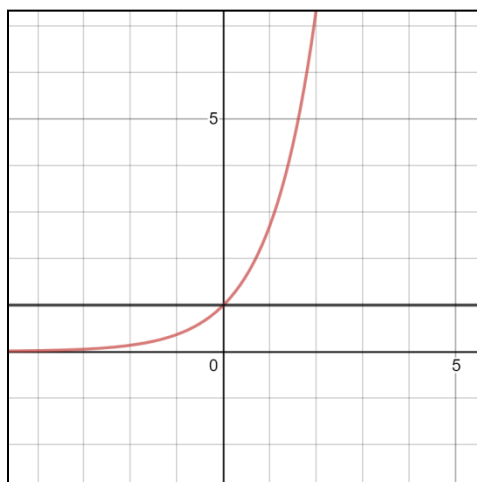


Figure 1

Figure 1 shows the Maclaurian Polynomial at a length of 1 term (Black Line) compared to the polynomial e^x .

Similarly

¹ A working animation for this Maclaurian series can be found at-
<https://www.desmos.com/calculator/xvfkxv7nng>

$$F'(0) = 1$$

$$P(0) = C_1$$

And so, $C_1 = 1$

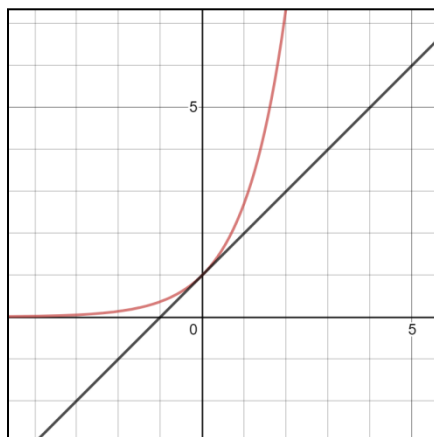


Figure 2

Figure 2 shows the Maclaurian Polynomial at a length of 2 terms (Black Line) compared to the polynomial e^x .

Matching all coefficients gives

$$C_0 = 1$$

$$C_1 = 1$$

$$C_2 = \frac{1}{2!}$$

$$C_3 = \frac{1}{3!}$$

$$C_4 = \frac{1}{4!}$$

Making

$$P(x) = 1 + \frac{x}{1!} + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!}, -\infty < x < \infty$$

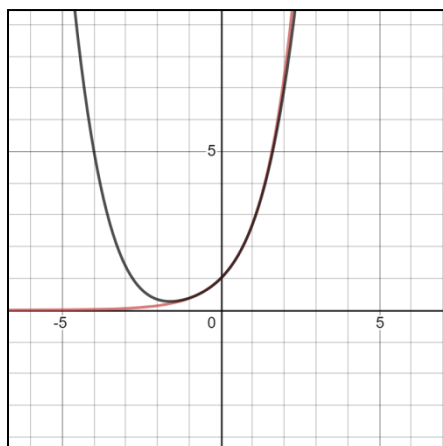


Figure 3

Figure 3 shows the Maclaurian Polynomial at a length of 5 terms (Black Line) compared to the polynomial e^x . One can observe how it gets more accurate as terms are added with the relevant coefficients.

As we add more terms, the series becomes a better approximation for $f(x)$ and hence, one can say that in the limit, $f(x) = P(x)$

Hence, one has approximated as such.

$$e^x = 1 + \frac{x}{1!} + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots, \quad -\infty < x < \infty$$

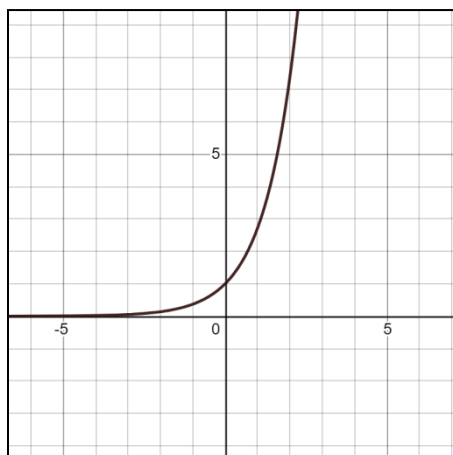


Figure 4

Figure 4 shows how accurate the Maclaurian polynomial is as an approximation of e^x at 50 terms.

One can form a general formula, for this process.

The Maclaurian Approximation for any function $f(x)$ is defined as

$$P(x) = f(a) + \frac{df(a)}{dx} \frac{x - a}{1!} + \frac{d^2f(a)}{dx^2} \frac{(x - a)^2}{2!} + \frac{d^3f(a)}{dx^3} \frac{(x - a)^3}{3!} + \dots, \quad -\infty < x < \infty$$

Where $a = 0$.

Similarly, one can express the following as Maclaurian Polynomial Series

$$\sin(x) = \frac{x}{1!} - \frac{x^3}{3!} + \frac{x^5}{5!} \dots, \quad -\infty < x < \infty$$

Where $f(x) = \sin(x)$ and $P(x)$ is the Polynomial.²

² A working animation for this Maclaurian series can be found at-
<https://www.desmos.com/calculator/oosxnh1h5r>

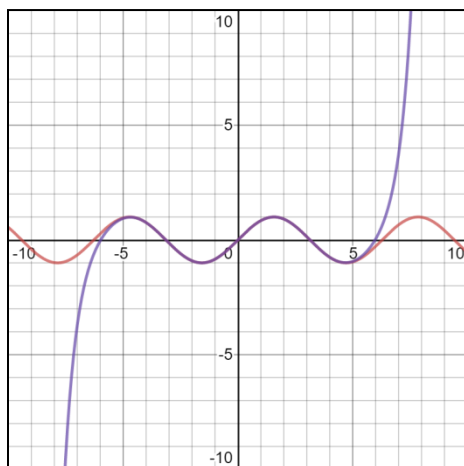


Figure 5

Figure 5 shows a Maclaurian expression for $f(x) = \sin(x)$ at 6 terms in length.

A working animation of this Maclaurian series can be found at-

And

$$\cos(x) = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} + \dots, \quad -\infty < x < \infty$$

Where $f(x) = \cos(x)$ and $P(x)$ is the Polynomial.³

³ A working animation of this Maclaurian series can be found at-
<https://www.desmos.com/calculator/qamvmqne6v>

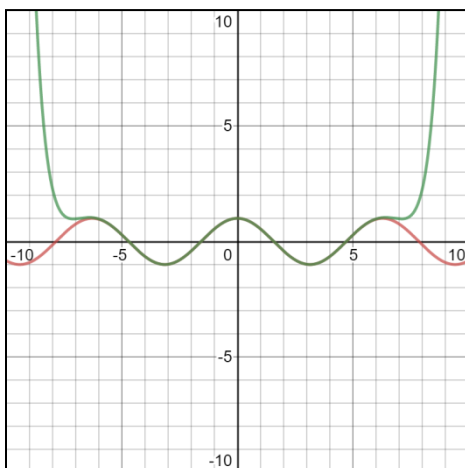


Figure 6

Figure 6 shows a Maclaurian expression for $f(x) = \cos(x)$ at 6 terms in length.

2.1.2) The $e^{\pi i}$ Transform and the Complex plane

If one considers the Maclaurian series of e^x .

$$e^x = 1 + \frac{x}{1!} + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots, \quad -\infty < x < \infty$$

One can consider the value of the function when $x = i\theta$

$$e^{i\theta} = 1 + \frac{i\theta}{1!} + \frac{(i\theta)^2}{2!} + \frac{(i\theta)^3}{3!} + \dots$$

Which can be expressed as, when i^2 is expressed as -1;

$$e^{i\theta} = 1 + \frac{i\theta}{1!} - \frac{\theta^2}{2!} - \frac{i\theta^3}{3!} + \dots,$$

$$e^{i\theta} = 1 - \frac{\theta^2}{2!} \dots + \frac{i\theta}{1!} + \frac{i\theta^3}{3!} + \dots,$$

Which can finally be rearranged as;

$$e^{i\theta} = \left(1 - \frac{\theta^2}{2!} \dots\right) + i\left(\frac{\theta}{1!} + \frac{\theta^3}{3!} + \dots\right)$$

When expressing as their respective Maclaurian series, we find that

$$e^{i\theta} = (\cos(\theta)) + i(\sin(\theta))$$

When plotted on an imaginary plane, one can observe how any value of theta corresponds to a point on the unit circle, defined by a real cosine component and an imaginary sine component.

One must notice, that when plugging in any value of θ , one can observe that the output always lies on the unit circle.

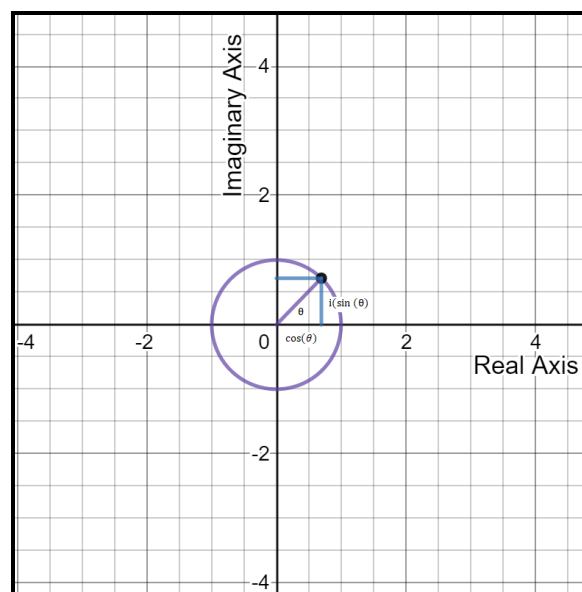


Figure 7

Figure 7: Shows the $e^{i\theta}$ transform, and how any $\cos(\theta) + i(\sin(\theta))$ can be expressed as a point on the unit circle. This has the effect of transforming any real number to a point on the unit circle.

*One can see, now, why the famous identity $e^{\pi i}$ corresponds to a walk of π radians around the circle, which equals -1 .*⁴

2.1.3) Fourier Transforms

There is perhaps no mathematical tool above that is as integral to this EE as the Fourier Transform. This will allow one to break up any wave function, into a series of sine waves, with different frequencies.

One can then determine the energies and frequencies associated with these waves.

The transform will be discussed in the next section on Math.

2.2) Physics and Chemistry Concepts required for the understanding of this investigation

2.2.0) Orbitals in atoms⁵

In atoms, electrons fill up orbitals (subshells), which are regions of space where they have a high probability of existing.

Each orbital can hold 2 electrons, so each orbital acts as a subshell for the shell which it is a part of. Since all orbitals hold the same amount of electrons, and all orbitals within the same shell therefore hold the same amount of energy (the energy of the electrons is determined by the shell) these all orbitals within a shell are called degenerate orbitals.

To maintain the lowest possible energy and so the most stable state, electrons fill up orbitals with lower energies first, given by a prescribed order in the Aufbau Principle, shown in Fig 1.

⁴ A working animation for the $e^{\pi i}$ transform can be found at- <https://www.desmos.com/calculator/tmhmc2z9oo>

⁵ Owen, Steve. "Bonding, Periodic Table and Infrared Spectroscopy." Chemistry for the IB Diploma. Cambridge: Cambridge UP, 2017. N. pag. Print.

The number of orbitals in a shell is prescribed by the number of electrons in each shell, given by the formula $2n^2$ where n is the shell number. For example, shell 2 has 8 electrons, which require 4 orbitals. This means that there is 1 s orbital and 3 degenerate p orbitals (p_x , p_y and p_z - Fig 3.) in shell 2.

Different orbitals come in different amounts. An S orbital is always singular. There are always 3 degenerate p orbitals and there are always 5 degenerate d orbitals (Fig 3).

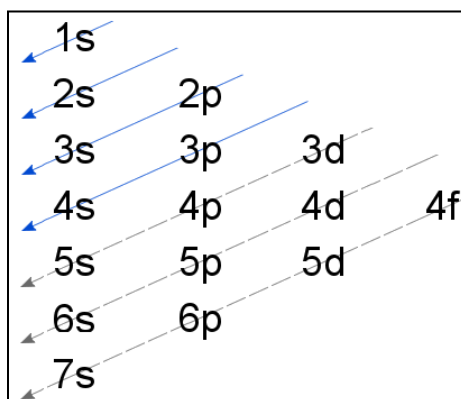


Figure 8

Figure 8: Orbitals are filled based on the Aufbau Principle, where orbitals of lower energy are filled first, as determined by the arrows in the diagram. This maximizes stability. In this case, the energies of the rows increase as one goes down the diagram (Hence the order of filling the orbitals follows 1s, 2s, 2p, 3s, 3p... etc.).⁶

⁶ Aufbau Principle. Digital image. N.p., n.d. Web. <<https://www.chemcool.com/definition/aufbau-principle.html>>.

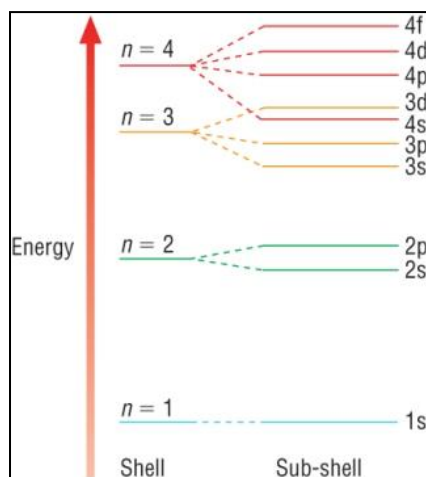


Figure 9

Figure 9: Shows the different orbital that act as subshells for each shell of an atom. Each orbital holds 2 electrons. This shows the energy of orbitals and hence shows why the Aufbau principle dictates that certain orbitals are filled before others.⁷

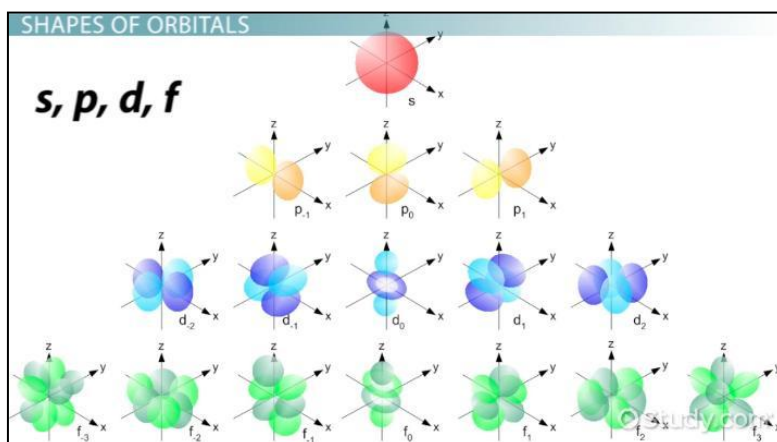


Figure 10

Figure 10: Shows the shapes of different orbitals and how many degenerate orbitals of each kind exist.⁸

When filling up orbitals, electrons obey 2 basic rules.

⁷ Energy Levels. Digital image. N.p., n.d. Web.

<http://www.chemhume.co.uk/A2CHEM/Unit%202b/11%20Transition%20elements/>.

⁸ Shapes of Orbitals. Digital image. N.p., n.d. Web. <https://study.com/academy/lesson/electron-orbital-definition-shells-shapes.html>.

a. The Pauli Exclusion Principle:

This states that 2 or more identical fermions cannot have the same spin in a quantum system.⁹

Hence, when filling up orbitals, electrons pair up, one with spin up and the other with spin down.

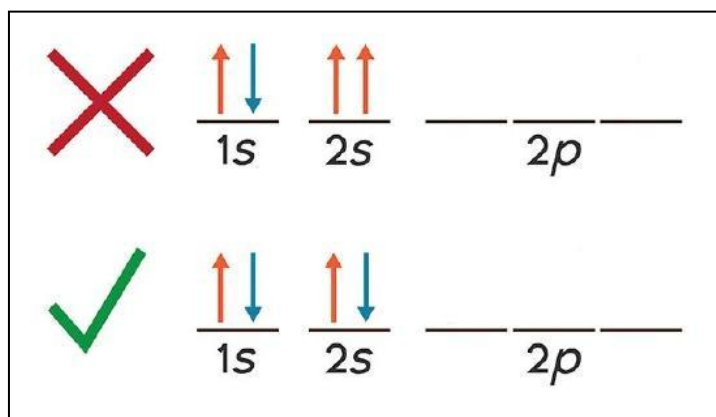


Figure 11

Figure 11: Shows how electrons in an orbital always pair up with one taking the form of spin up (upward arrow) and the other with spin down (downward arrow). This is done to minimize electron repulsion in orbitals and hence maximize stability.¹⁰

b. Hund's Rule:

Hund's Rule follows that electrons must minimize the energy of their system to maximize stability. Hence, they occupy different orbitals until it is necessary to pair up. Hence, we observe that every suborbital is singly filled before any pairing occurs.

⁹ Spin is defined as an electromagnetic property intrinsic to any quantum particle.

¹⁰ Pauli Exclusion Principle. Digital image. N.p., n.d. Web.

<[https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Supplemental_Modules_\(Physical_and_Theoretical_Chemistry\)/Electronic_Structure_of_Atoms_and_Molecules/Electronic_Configurations/Pauli_Exclusion_Principle>](https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Supplemental_Modules_(Physical_and_Theoretical_Chemistry)/Electronic_Structure_of_Atoms_and_Molecules/Electronic_Configurations/Pauli_Exclusion_Principle>)

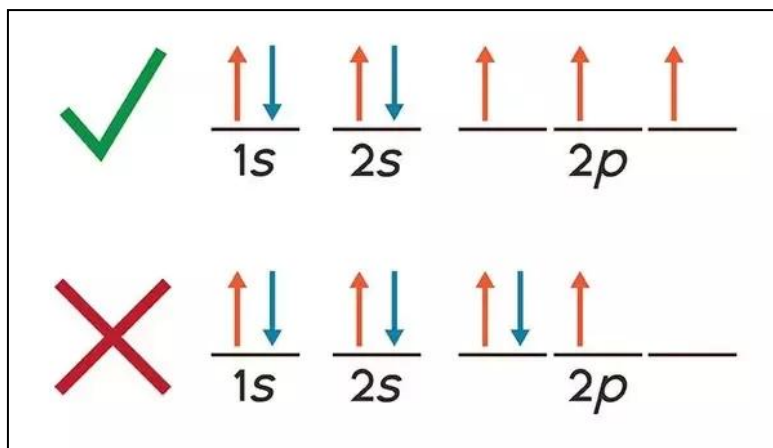


Figure 12

Figure 12: Shows how electrons always singly fill up degenerate orbitals before pairing up in a single orbital. This is done to minimize repulsions and maximize the stability of the atom. ¹¹

2.2.1) The energy of an electron in an orbital^{12,13}

One must know how one can obtain the energy of an electron. To do so, one must understand how term symbols. These are simple sets of notation, used to describe the system in which the electron is a part of.

The term symbol is given by J, and this can be calculated using Hund's rules.

To find J, one must define 2 other values, L and S.

L is the sum of all the m_l values for electrons in the orbital. The m_l value is given to an electron based on its degenerate orbital. These values are spread equally around 0.

¹¹ Hund's Rule. Digital image. N.p., n.d. Web. <<https://www.quora.com/Why-does-platinum%E2%80%99s-electron-configuration-not-conform-to-Hund%E2%80%99s-rule-i-e-have-a-full-5D-orbital-as-other-metals-in-its-group-do-e-g-palladium>>;

¹² "Atomic Spectra Database - Energy Levels Form." *NIST*. N.p., n.d. Web. 23 Sept. 2019. <https://physics.nist.gov/PhysRefData/ASD/levels_form.html>.

¹³ "Term Symbol." *1925ApJ....61...38R Page 38*. N.p., n.d. Web. 23 Sept. 2019. <<http://adsabs.harvard.edu/full/1925ApJ....61...38R>>.

For example, a p orbital holds 6 electrons, and hence has 3 degenerate orbitals. This means that each of these orbitals have ml values of 1, 0 and -1 respectively.

Each electron in any degenerate orbital attains the ml value of the degenerate orbital it is a part of.

S is the sum of all the spins of all the electrons. As leptons, all electrons have a spin of ± 0.5 .

Due to Hund's rule, electrons singly fill up individual orbitals and hence, have the same spin, before following the Pauli Exclusion Principle and pairing up 2 electrons in one orbital.

Now, with values for L and S, one can calculate J as-

Less than half of the subshell is occupied	More than half-filled	The subshell is half-filled
Take the minimum value $J = L - S $	Take the maximum value $J = L + S;$	Then L will be 0, so $J = S.$

An example: Carbon's P orbital.

Carbon's p orbital holds 2 electrons. Which means they both have the same spin, and occupy 2 of the 3 available degenerate p orbitals- p_x , p_y or p_z . Since the orbital is less than half full

$$J = |L - S|$$

Minimum value of L	Minimum value of S	J value
-1	0	1

$$J = |-1 - 0|=2$$

The term is $^{2S+1}(\text{Orbital})_J$

Hence, the term of the energy in a carbon p orbital is 3P_1

Now, one can obtain the data associated with an electron with this term using online resources.

The electrons wave number ($1/\lambda$) is given by 43.41350 cm^{-1} .¹⁴

From which one can determine λ , and hence the frequency of the associated wave using the equation $c=f\lambda$, where

Symbol	Meaning
C	Speed of light
Λ	Wavelength of the wave
F	Frequency of the wave

2.2.2) Infrared Spectroscopy- the energy of a bond.

Infrared Spectroscopy is a technique used to determine the strength of a bond. The strength of a bond is the amount of energy required to break it by causing the electrons to get so excited that they escape the bond with the gained energy, breaking it.

Since the understanding of this process is not integral to the investigation, it has not been explained in detail.

2.2.3) Plank's Equation¹⁵

Plank's equation is essential to this Essay, as it allows one to convert from an energy, to an associated wave.

¹⁴ "Energy Levels of Electrons in Orbitals." *Energy Levels of Neutral Carbon (C I)*. N.p., n.d. Web. 22 Sept. 2019. <<https://physics.nist.gov/PhysRefData/Handbook/Tables/carbontable5.htm>>.

¹⁵ Tsokos, K. A. "Quantum Phenomena- Plank's Equation." *Physics for the IB Diploma*. Cambridge: Cambridge UP, 2016. N. pag. Print.

Fourier transforms are involved with the addition and resolution of waves, and hence, the equation allows one to convert any energy to wave form, allowing for one to apply the Fourier Transform.

$$E = hf$$

Symbol	Meaning
E	Energy
H	Plank's constant
F	Frequency of the wave

2.2.4) Hybridization Theory¹⁶

One can observe that atoms like carbon regularly form 4 bonds, which have equal energy. Carbon does not possess 4 valence electrons of equal energy as it possesses 2 2s electrons (with less energy that are filled initially as mentioned above) and 2 2p electrons. Still, we observe that all carbon bonds have the same energy using Infrared spectroscopy. The explanation provided for such phenomenon, is called hybridization theory.

Hence, one can observe hybridization theory, which states that electrons in the s orbital and the 3 p orbitals mix to form 4 sp³ orbitals and hence, obtain a middle ground where they all have the same amount of energy, similar to mixing paint in a can.

In the case of carbon, the 1 s orbital and 3 p orbitals which hold 2 and 2 valence electrons mix to form 4 new sp³ orbitals, shaped in a tetrahedron, of equal energy, which each hold 1 electron, and are used for bonding.

¹⁶ Brown, Catrin, and Mike Ford. "Bonding- Hybridization." *Higher Level Chemistry*. Harlow, Essex: Pearson Education, 2014. N. pag. Print.

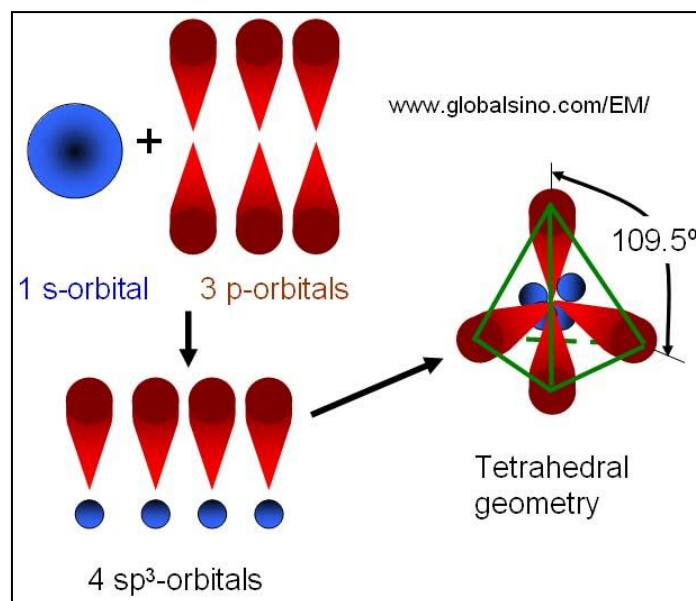


Figure 13

Figure 13: Shows how hybridization occurs in the case when 1 $2s$ and 3 $2p$ orbitals mix to form 4 sp^3 orbitals of equal energy, which take up a specific geometry to minimize electron repulsions and maximize stability. These 4 hybrid orbitals, with the same energy, can all form bonds of equal strengths with other atomic orbitals.¹⁷

The theory also allows one to predict the orientation and shape of these new hybrid orbitals. This is done by accounting for the fact that electrons minimize repulsions amongst each other to form a system with the lowest energy (more stable).

One can derive this. If the force on each electron on another is given by Coulombs law, this, however, is not relevant to the investigation.

¹⁷ Hybridization Theory. Digital image. N.p., n.d. Web. <<http://www.globalsino.com/EM/page2118.html>>.

3.0) Using Math to develop the model^{18,19}

One can begin to understand the Fourier Transform when considering a mixed wave, a sum of different sine waves.^{20,21}

Let us consider the wave, $f(x)$, as a sum of sine waves.

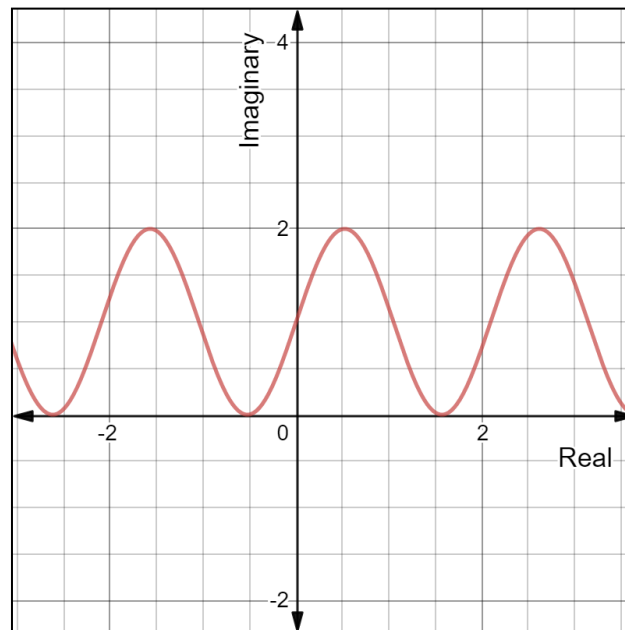


Figure 14

Figure 14 shows the wave $f(x)$, which is about to be subject to the Fourier Transform.²²

When multiplied by $e^{\pi i}$, one can plot the wave on a complex plane, where the wave has essentially been wrapped around the origin.

Let us called this transformed wave $g(x)$

¹⁸ An animation that ties all the images together can be found at-
<https://www.desmos.com/calculator/oikh4zpk3>

¹⁹ Cheever, Erik, and Swarthmore College. "Introduction to the Fourier Transform." *Linear Physical Systems - Erik Cheever*. N.p., n.d. Web. 22 Sept. 2019. <<https://lpsa.swarthmore.edu/Fourier/Xforms/FXformIntro.html>>.

²⁰ Bevelacqua, Pete. "Fourier Transforms." *Fourier Transform*. N.p., n.d. Web. 22 Sept. 2019.
 <<http://www.thefouriertransform.com/>>.

²¹ "Fourier Transform." *From Wolfram MathWorld*. N.p., n.d. Web. 22 Sept. 2019.
 <<http://mathworld.wolfram.com/FourierTransform.html>>.

²² NOTE: In images displayed below, the graph being used is not a sum of sine waves, rather, a single sine wave. The following example goes through the same process with a sum of sine waves.

We can say that

$$g(x) = f(x)e^{2\pi ix}$$

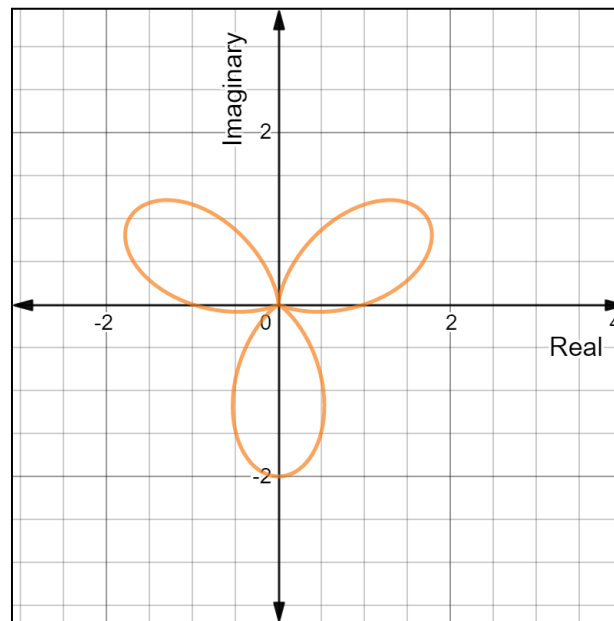


Figure 15

Figure 15 shows the same wave $f(x)$, but wrapped around the origin as the $e^{\pi i}$ transform (discussed above and in background information) is applied.

The 2 was added before the transform to make sure that one completes a full circle. This is done as 2π radians can be travelled to wrap the wave all around the origin. This means that currently, moving forward 1 unit along the wave corresponds to moving around the origin exactly once, as 2π have been covered.

The distance of $f(x)$ from the origin is determine solely by the height of $g(x)$ at a point, as the $e^{\pi i}$ transform allows one to wrap to a unit circle.

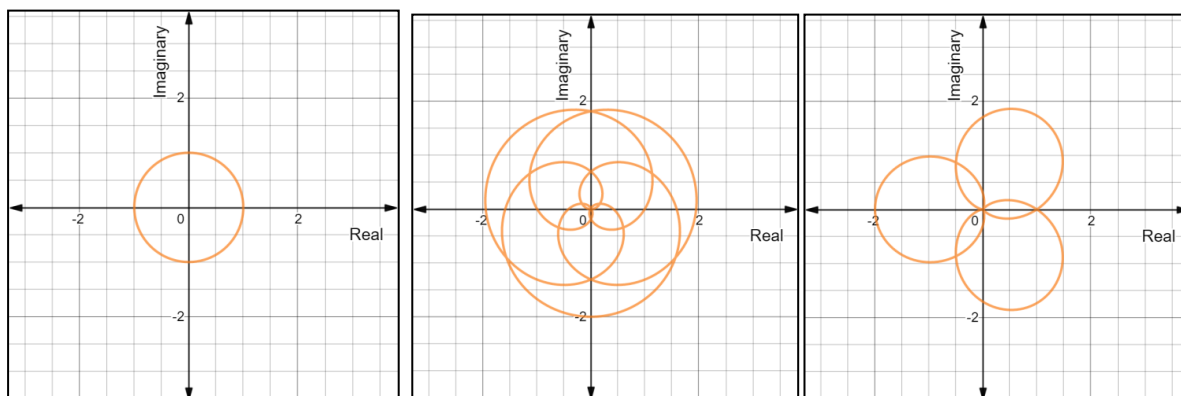
High points on $f(x)$ correspond to points on $g(x)$ further away from the origin, and low points correspond to points closer to the origin.

The key point that one can make, is introduce a new variable, that allows one to control, how fast exactly, $f(x)$ is wrapped around the origin. The introduction of this variable makes the new function $g(x)$

$$g(x) = f(x)e^{2\pi i\omega x}$$

Where ω describes how fast the graph is wound around the origin. Changing the value of ω makes it so that the graph looks very different. For example, if the value of ω was changed to $1/10$, the graph would now make a revolution of 2π radians in 10 x-units instead of 1.

The graphs below showcase the same wave with different winding frequencies ω



<u>Figure 16</u>	<u>Figure 17</u>	<u>Figure 18</u>
$\omega = 0$	$\omega = 0.2$	$\omega = 0.5$

Figures 16, 17 and 18: Show how a changing value of ω affects how the wound up graph looks.

A negative sign is introduced into the function, to represent the fact that the wrapping of the wave occurs in the anti clock wise direction. This is simply notational.

$$g(x) = f(x)e^{-2\pi i\omega x}$$

This expression encapsulates the idea of wrapping $f(x)$ around the origin with a variable speed with how much it is wrapped.

What one must now do is track the centre of mass of the wound up graph. How one may do this, is by adding multiple instances of the graph, as complex numbers, and then dividing by the number of points added.

This can be represented by the equation

$$g(x) = \frac{1}{N} \sum_{x=1}^N f(x) e^{-2\pi i \omega x}$$

N represents the number of points being added together as complex numbers. When divided by N , one would obtain an average, which would represent the centre of mass of the system.

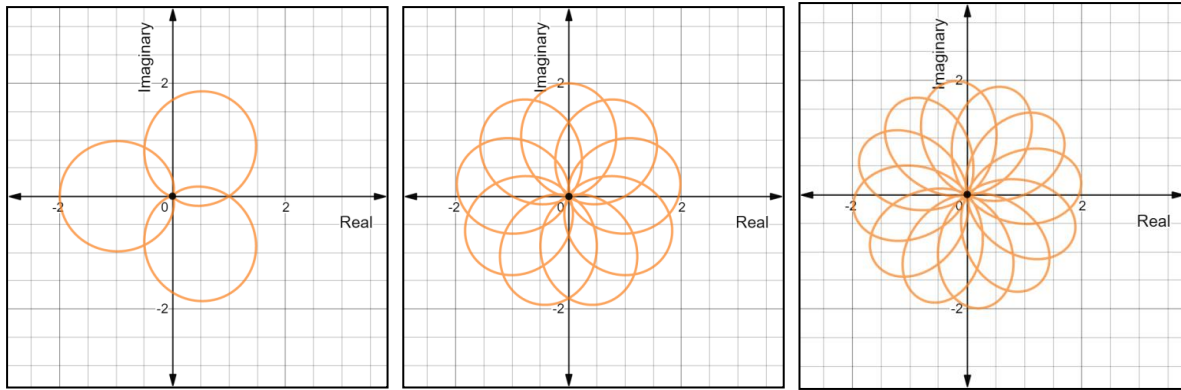
This function would become more accurate as N increases. Hence, letting it tend to infinity,

$$g(x) = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{x=1}^N f(x) e^{-2\pi i \omega x}$$

Gives the following equation.

$$g(x) = \frac{1}{x_2 - x_1} \int_{x_1}^{x_2} f(x) e^{-2\pi i \omega x} dx$$

Hence, one has built an equation for $g(x)$, which gives how far the centre of mass is from the origin, for any wave $f(x)$, when wound about the origin at a frequency of ω cycles per unit.



<u>Figure 19</u>	<u>Figure 20</u>	<u>Figure 21</u>
$\omega = 0.5$	$\omega = 0.6$	$\omega = 0.8$

Figures 19, 20 and 21: Show the centre of mass (marked as the black point) of wound up graphs of $f(x)$ with different values of ω

A key point to note, is when the frequency of winding, ω , matches the frequency of one of the constituent waves of the graph. Now, all the crests of the wave line up at a point (above origin), and the centre of mass shifts, giving a higher reading than natural. Hence, by observing the distance of the centre of mass from the origin, one can tell the frequencies of the waves that constitute the superimposed wave.

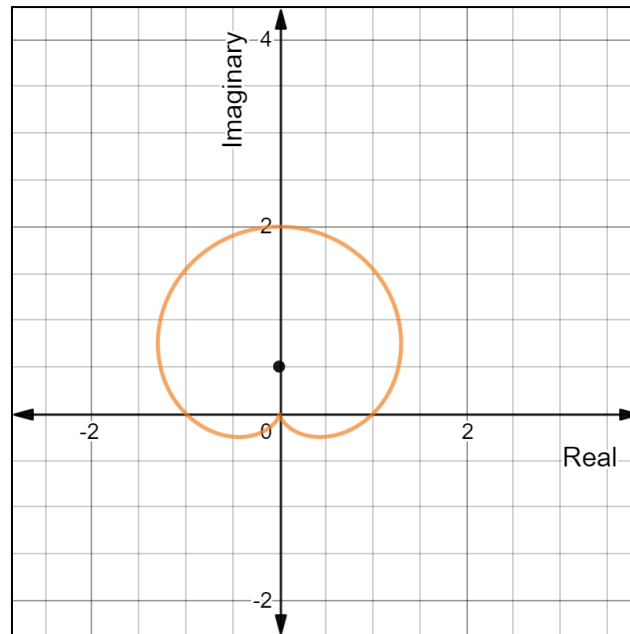


Figure 22

Figure 22: Shows how when the winding frequency matches the frequency of the wave, the crests line up at one point around the origin which leads to a shift of the centre of mass away from the origin.

This is almost the Fourier Transform.

For a real Fourier transform, one doesn't divide out by the x interval. This corresponds to the fact that instead of looking at the centre of mass of the system, the value is scaled up by some amount.

$$g(x) = \int_{x_1}^{x_2} f(x)e^{-2\pi i\omega x} dx$$

If the portion of the graph being analyzed is of a time interval of k, the value is scaled up by k.

This has the effect of the longer a frequency persists, the larger the magnitude of the Fourier Transform is- letting one establish the weightage constituent wave as a part of the superimposed function.

This accentuates the effect that the centre of mass, for a larger x interval is more likely to show a higher value when the winding frequency matches the frequency of one of the constituent waves of the function, and for all other points, the small distance of the centre of mass from the origin cancels this out, leaving a value of near zero.

One can plot the values of ω on the x -axis and the distance of the centre of mass from the origin on the y axis.²³

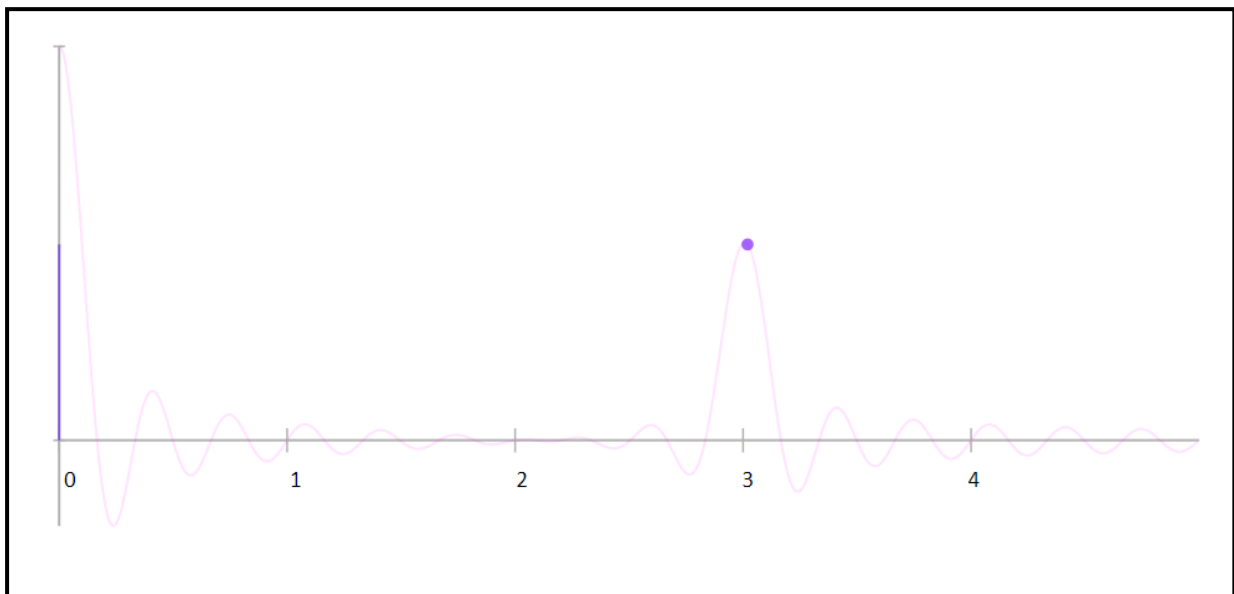


Figure 23

Figure 23 plots the values of ω on the x axis and the distance of the centre of mass on the y axis. One can clearly see the peak marked by a jump, hence indicating that the original frequency of the graph is given by 3. This was the frequency used in the example for $f(x)$.

²³ DSouza, Prajwal. "Fourier Transform Visualization." *Fourier Transform Visualization*. N.p., n.d. Web. 22 Sept. 2019. <<https://prajwalsouza.github.io/Experiments/Fourier-Transform-Visualization.html>>.

If a certain constituent wave makes up k times of another, the centre of mass shifts away from the origin by approximately k times, as k times as many crests of the weighted wave have aligned to cause this shift. This is useful when it comes to mixing multiple of one wave to form another. This will be witnessed in the next example.

Example: An application to a theoretical model of hybridization- sp^3 hybridization.²⁴

Let us consider

$$f(x) = \sin(x) + 3\sin(3x)$$

This represents the frequencies of electrons in 1 s orbital and 3 p orbitals, which mix to give an energy wave of 4 sp^3 hybridized orbitals.

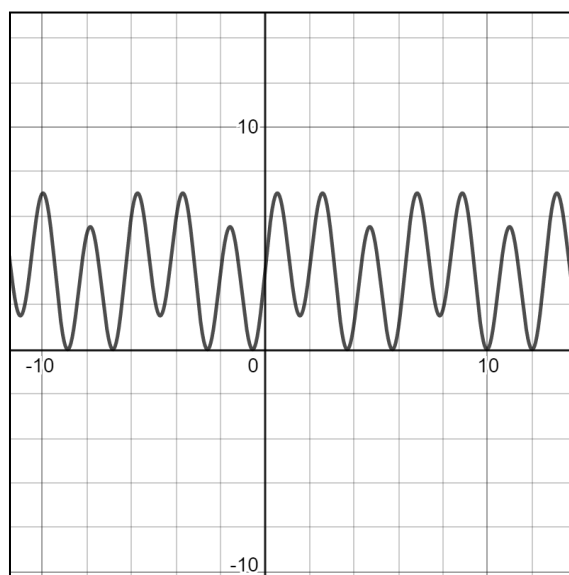


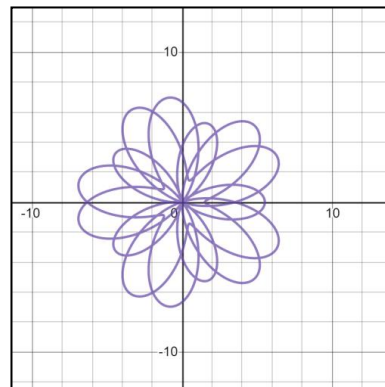
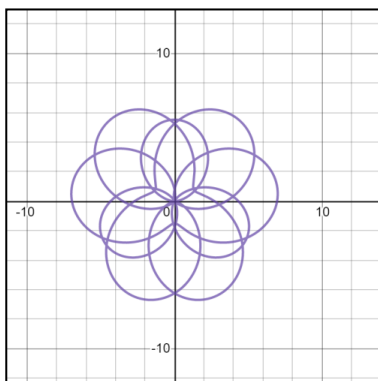
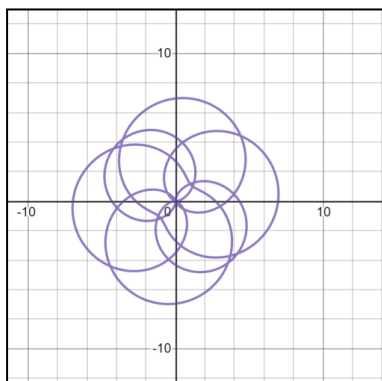
Figure 24

Figure 24: Shows the wave $f(x)$ which represents the mixing of 1 s orbital and 3 p orbitals, which mix to give an energy wave of 4 sp^3 hybridized orbitals.

One can use the Fourier transform to wrap this function around the origin as such.

²⁴ The graphs for the example, with included animations for visualization, can be found at- <https://www.desmos.com/calculator/zljej58apt>

$$g(x) = f(x)e^{-2\pi i\omega x}$$

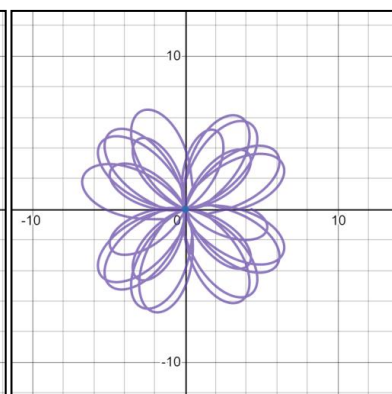
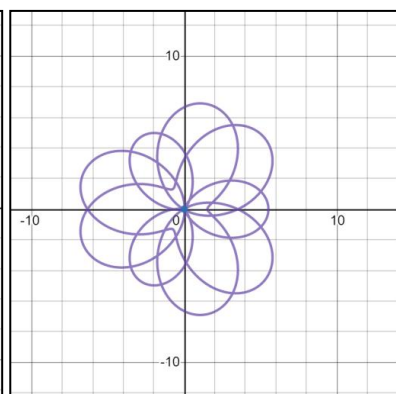
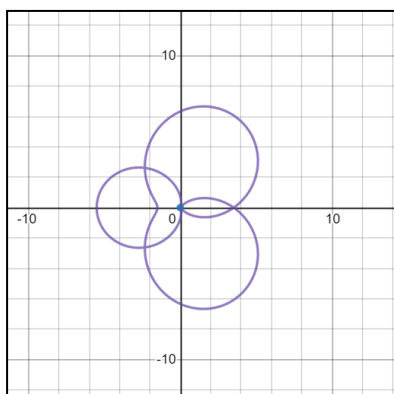


<u>Figure 25</u>	<u>Figure 26</u>	<u>Figure 27</u>
$\omega = 0.4$	$\omega = 0.6$	$\omega = 1.25$

Figures 25, 26 and 27: Show how the wound graph of $f(x)$ around the origin changes for different values of ω . This was done by applying the $e^{\pi i}$ transform.

And then find the wrapped function's centre of mass.

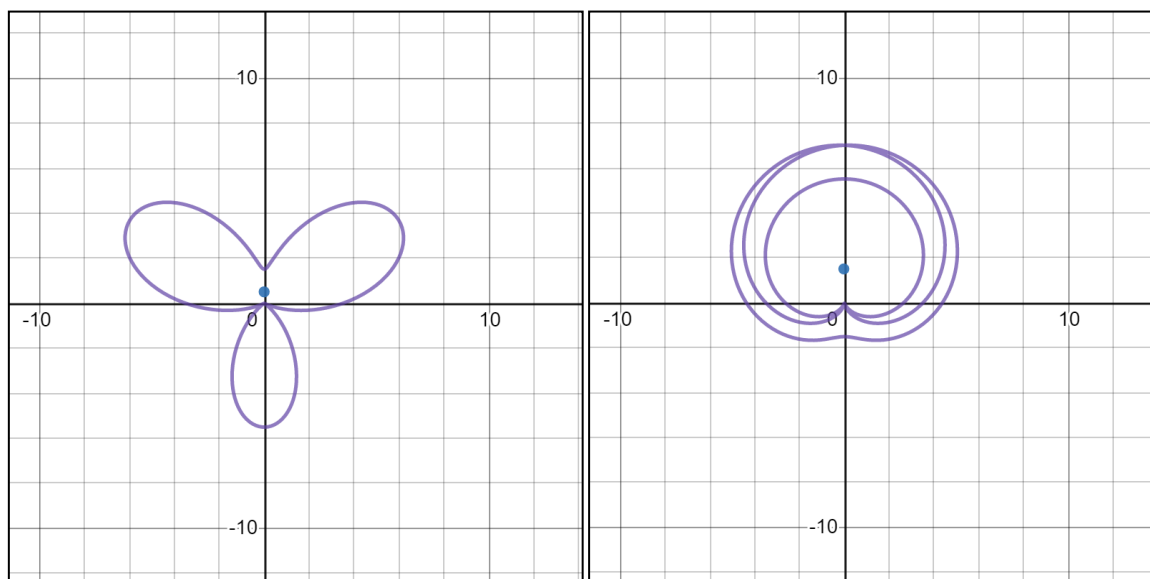
$$g(x) = \int_{x_1}^{x_2} f(x)e^{-2\pi i\omega x} dx$$



<u>Figure 28</u>	<u>Figure 29</u>	<u>Figure 30</u>
$\omega = 0.5$	$\omega = 0.75$	$\omega = 1.3$

Figure 28, 29 and 30: Show the centre of mass (defined as the blue marked point), for the wound graph of $f(x)$ around the origin for different wrapping frequency values of ω , when the $e^{\pi i}$ transform was applied.

Then, by changing the value of ω one can observe when the value of the centre of mass increases. This occurs when ω takes the values of the frequencies of the original constituent sine waves, 1 and 1/3 respectively.



<u>Figure 31</u>	<u>Figure 32</u>
$\omega = 1$	$\omega = 0.3333$

Figures 31 and 32: Shows the position of the centre of mass (shifted away from origin) when the value of ω reaches 1 and 1/3, the values of the frequencies of the constituent sine waves that make the function $f(x)$, which was wrapped around the origin by the $e^{\pi i}$ transform.

One can note how the centre of mass of the wound wave shifts away from the origin when the winding frequency ω matches the frequencies of the constituent sine waves of $f(x)$ because at these frequencies the crests of the waves align at one point above the origin and the troughs align at the bottom, creating a shape with a shifted centre of mass.

The distance of the centre of mass from the origin increases as ω reaches 1 and 1/3, the amount the centre of mass shifts when the value of ω reaches 1/3 is approximately 3 times the shift when ω reaches 1.

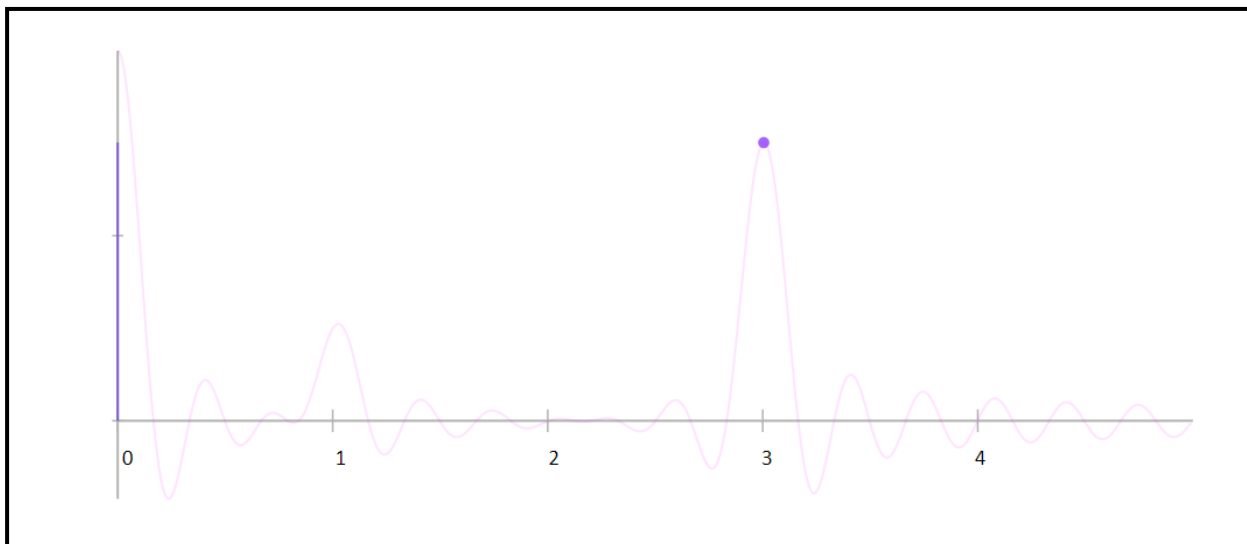


Figure 33

Figure 33 plots the values of ω on the x axis and the distance of the centre of mass on the y axis. One can clearly see the peaks marked by jumps in the graph; indicating that the original frequencies of the sine waves are given by 1 and 3.

One can also note that there were 3 waves of frequency 3, when ω reaches 3, the jump is about 3 times as large as when ω equals 1.²⁵

This informs one about the fact that 1 wave of frequency 1 and 3 waves of frequency 3 have are constituent elements of the mixed wave that was inputted into the transform.

²⁵ DSouza, Prajwal. "Fourier Transform Visualization." *Fourier Transform Visualization*. N.p., n.d. Web. 22 Sept. 2019. <<https://prajwalsouza.github.io/Experiments/Fourier-Transform-Visualization.html>>.

4.0) Application of the Model

From theory in hybridization, the waves associated with orbital energies are added using a Fourier transform, the resultant wave will, post modulation (so that one can associate a single frequency to it), mirror the frequency of a hybrid orbital formed by the orbitals.

We will need data on the energy associated with the orbital of an atom, which can be obtained by first calculating the J term of the particular orbital, and then finding the associated wave number from online, as discussed in the section on background information (Energy of an electron in an orbital).

One can find the wavelength from the wavenumber, taking SI units, one can find the frequency of the wave.

$$c = f\lambda$$

Where

Symbol	Meaning
c	Speed of light
λ	Wavelength of the wave (determined using infrared spectroscopy- refer to background information)
f	Frequency of the wave

To determine the energy of the electrons part of the bond.

The energies of the resultant bonds that are expected from the Fourier Transform are obtainable from infrared spectrochemical data, of compounds that have the particular bond (with the correct hybridization type) present in them.

Example: sp^3 Hybridization of Carbon^{26,27}

The function is a sum of 1 2s orbital energy and 3 2p orbitals. This forms 4 sp^3 orbitals.²⁸

The frequency of the electron in the 1 2s orbital is given as- 6.49×10^{14} Hz

The frequency of the electron in the 3 2p orbital is given as- 1.3039×10^{12} Hz²⁹

When plotted,

$$f(x) = \sin(0.154x) + 3\sin(0.00718x)$$

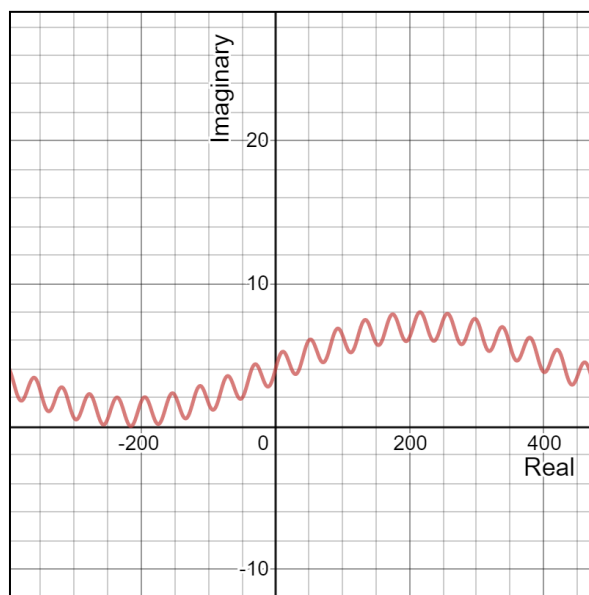


Figure 34

²⁶ The graphs for with this animation can be found at-

<https://www.desmos.com/calculator/mq1xa3enyk>

²⁷ NOTE: In this example, frequencies are extremely high, and hence, have been shifted to a more convenient scale by dividing by a constant for all frequencies.

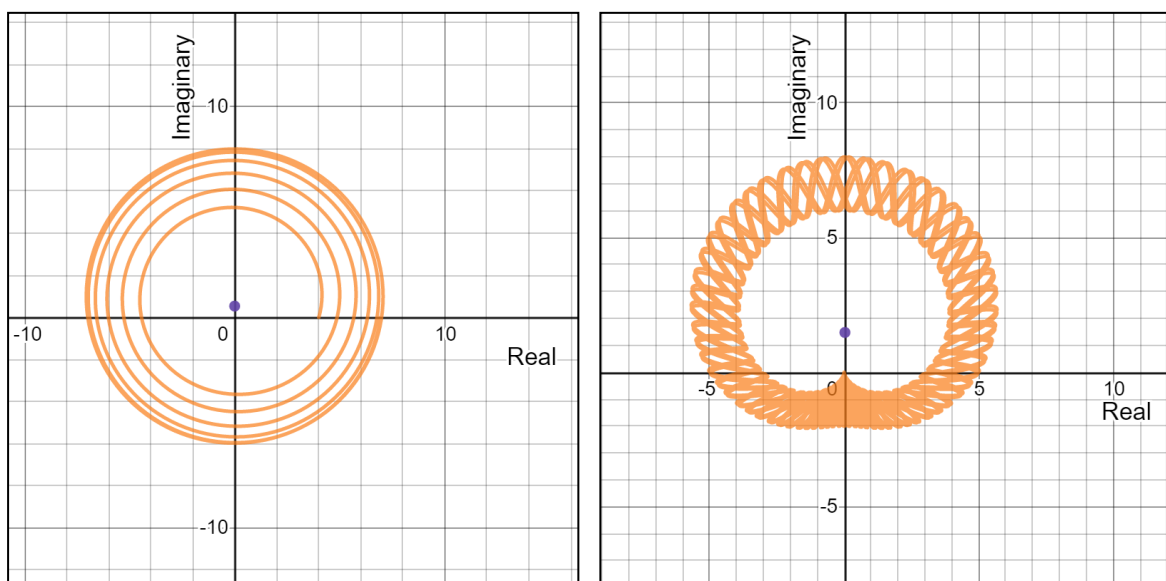
²⁸ NOTE: This data was obtained from online, where J values were calculated (as discussed in the background information section), and wave numbers and hence frequencies deduced. It should also be noted, that this constant is the same for all pieces of information for an example, but is not the same for all examples.

²⁹ "Energy Levels of Electrons in Orbitals." *Energy Levels of Neutral Carbon (C I)*. N.p., n.d. Web. 22 Sept. 2019. <<https://physics.nist.gov/PhysRefData/Handbook/Tables/carbontable5.htm>>.

Figure 34: Shows the graph of $f(x)$ which represents the mixing of 1 s orbital and 3 p orbitals, which mix to give an energy wave of 4 sp^3 hybridized orbitals in relation to a carbon atom.

The graph can be wound around the origin and its centre of mass observed.

When the Fourier transform is applied, one can see that the frequencies of the constituent waves are clearly seen.



<u>Figure 35</u>	<u>Figure 36</u>
$\omega = 6.49$	$\omega = 139.275$

Figures 35 and 36: ω reaches 6.49 and 139.275, the values of the frequencies of the constituent sine, which was wrapped around the origin by the $e^{\pi i}$ transform, with a winding frequency of ω .

The centre of mass of each wave is shifted off as the frequencies of one of the constituent waves causes the alignment of all the crests of the wave on one side and so, changes the centre of mass of the wound graph.

When modulated, the graph comes to

$$f(x) = 4\sin(0.007x)$$

Which models the graph of 1 resultant orbital, with increased amplitude.

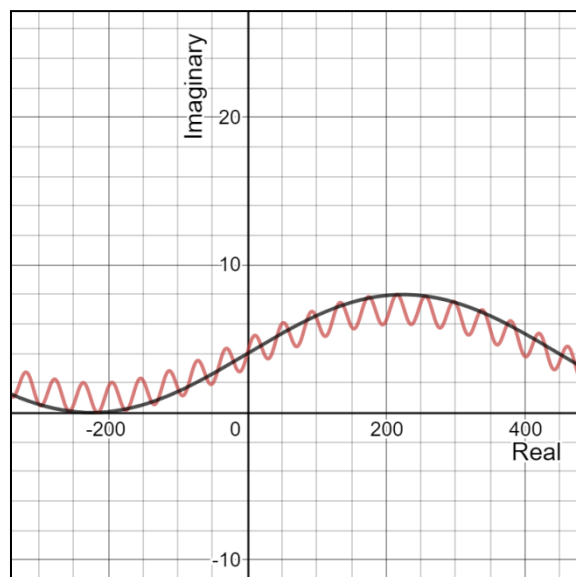


Figure 37

Figure 37: Shows a modulated version of the mixed graph of $f(x)$.

To bring the amplitude back to 1, and so, control for the energy, one must mix 4 of the previous sin waves to form 1 wave with 4 times the frequency.

$$F(x) = \sin(0.028x)$$

This wave holds the same energy as the waves obtained from the Fourier transform, only modulated with 1 frequency and amplitude of 1.

Secondly

One can observe, from the spectrochemical data of ethane (which contains a single C-C bond involving 2 sp^3 orbitals), with a frequency of 0.36×10^{14} Hz.

A graph that represents this is given by ³⁰

$$G(x) = \sin (0.0277x)$$

Which is extremely similar to the modulated graph observed through the addition of 1 2s and 3 2p orbitals, which are the orbitals that constitute a sp^3 orbital.

$$F(x) \approx G(x)$$

Indicating that the theory has correctly predicted the hybridization of carbon.

The theory was applied to different complexes to check for consistency.

Sr No.	Hybridization	Element ³¹	Orbitals Involved	F(x)	G(x)	Similarity Factor R (0 to 1) ³²
1	sp^3	Carbon	1 2s orbital + 3 2p orbitals = 4 sp^3 hybrid orbitals	$\sin (0.0280x)$	$\sin (0.0277x)$	0.989
2	sp^2	Boron	1 2s orbital + 2 2p orbitals = 3 sp^2 hybrid orbitals	$\sin (0.0060x)$	$\sin (0.0066x)$	0.909
3	sp^3d	Nitrogen	1 2s orbital + 3 2p orbitals + 1 d orbital = 2 sp hybrid orbitals	$\sin 0.0060(x)$	$\sin (0.0055x)$	0.909

³⁰ "Ethane." *Ethane*. National Institute of Standards and Technology, n.d. Web. 22 Sept. 2019. <<https://webbook.nist.gov/cgi/cbook.cgi?ID=C74840&Type=IR-SPEC&Index=0>>.

³¹ NOTE: All compounds being considered are the element in a naturally occurring element. The elements are not integral to the nature of the math of the investigation and hence, not mentioned. The data of the G(x) was obtained from the respective infrared spectra of the compounds.

³² NOTE: The similarity factor is calculated by taking the difference in the frequencies and dividing by the expected frequency, hence giving the complement of the percentage of error. A similarity factor closer to 1 indicates better similarity as 1 indicates perfect similarity. Factors closer to 1 indicate the model gives a good prediction that fits reality well.

4.1) Analysis

The previous section showed that Fourier transforms could be used to break down a wave, and if appropriate waves that represented orbitals were added (using the transform), one could, modulate the resultant function and predict the hybridization that would occur.

Results were fairly accurate to reality, with similarity values of 0.989, 0.909 and 0.909 for the 3 tested hybridization types. These were calculated in the section above.

The following sections will evaluate different aspects of the model.

4.2) Assumptions

1.) An assumption made is that all data was collected from the same source, by the same chemists, at the same conditions. Different conditions (like temperature, pressure etc.) would change the behaviour of the atoms and the observed values.

This is the probable reason behind the similarity values not being a perfect 1 or the predicted values deviating a little from reality.

This however, is hard to account for and makes the process a lot more tedious. One could attempt this with the appropriate infrastructure (which was not available during this investigation), obtain all the values with appropriate controls and get better results. Errors in data collection are a significant factor and have possibly been responsible for the deviations noticed here.

4.3) Strengths

1.) The model is a good fit, and its predictions have high similarity values to reality-, which makes it a good predictor of the hybridization of complexes. This means that the model, is useful and possibly reflects reality well.

2.) As a simpler model as compared to models that achieve the same purpose, it requires less cognitive strain to understand- making an excessively complicated model, as explanation does not achieve the purpose of the model. A simpler model is more accessible.

However, models like the Schrodinger wave function predict more than what this model does and in better ways, and hence are essential to our understanding of reality.

3.) Many types of hybridization were predicted well by the model (sp^3d , sp^2 and sp^3). While there are other forms of hybridization, the models accurate prediction for these 3 types lend it credibility and help establish it's reliably results.

4.4) Weaknesses and Improvements

1.) During the investigation, not many data points being considered opens the theory up to random errors and reduced the reliability of the model. This cripples the generalizability of the investigation.

Generalizability and reliability is easily improved by considering more data points.

2.) The wave being modulated was the only way to check if it fits reality. The obtained wave, in reality, is a single frequency wave (as only 1 wavelength of light is absorbed during the infrared spectroscopy process.). This cripples the significance of the investigation, as a major use of the investigation allows one to predict hybridization of complexes by applying the process in reverse. This is discussed further in the implications section.

3.) Predictions made are not perfect ($|R| \neq 1$) indicating, that there are aspects of reality, that the model does not account for. This shows that, like most models, there are assumptions that do not reflect the reality of the situation.

4.5) Implications

The investigation provides an easier way to determine the hybridization of a complex. One must keep in mind, that unmodulating a wave is hard to do, and requires technology, but if this can be done, the frequency of any associated electrons in an orbital can be unmodulated and have a Fourier transform applied to determine the frequency of the constituent orbitals.

Hence, one can predict the hybridization of a complex.

5.0) Conclusion

Models are tools that we use to help explain and find patterns in reality with. That being said, no model can perfectly explain reality, and will have a limited domain. The model in consideration, does explain certain aspects of hybridization well, but not perfectly and is open to falsification.

When developing models, complexity is a major factor to consider. As a tool to explain more complicated situations, one may have to introduce detail and complexity. That being said, one must be wary not to make the model too complex, defeating its purpose by making it complicated. The key, is finding a middle ground, when the model fits reality well, but is also fairly easy to understand.

In the context of the Fourier transform, while the model does not explain many aspects of the atom like maybe Schrödinger's equation or others may, it is significantly simpler to understand and hence does have some usage in explanation. In understanding how hybridized orbitals obtain their energies, the model fits well, and is simple enough to understand. With this, one can conclude that it does achieve its purpose- explaining an aspect of reality.

6.0) Extensions and Other Applications

Fourier Transforms are extremely powerful mathematical tools, which allow for the deep analysis of waves. They can be used in multiple contexts.

1. The theory can be extended to bonding theory, and check if the addition of the energies of a 2 pi bonds and a sigma bond accurately predict a triple bond or such with a double bond.

2. A similar application of this theory can be conducted in determining the frequencies of notes played by musical instruments, and the mixing of these frequencies to make chords.

The Fourier transform can be helpful in investigating music with measure theory, about how notes mix to form pleasant or unpleasant sounds.

One could possibly explore Inverse Fourier Transforms used to remove certain frequencies by removing selected constituent waves from the transform.

3. Fourier Transforms are also used in Spectral and Frequency analysis in image transforms, to decompose images into sine and cosine components, and transmit them.

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