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Enhanced Quantum Chemistry With Machine Learning

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Enhanced Quantum Chemistry with Machine Learning.

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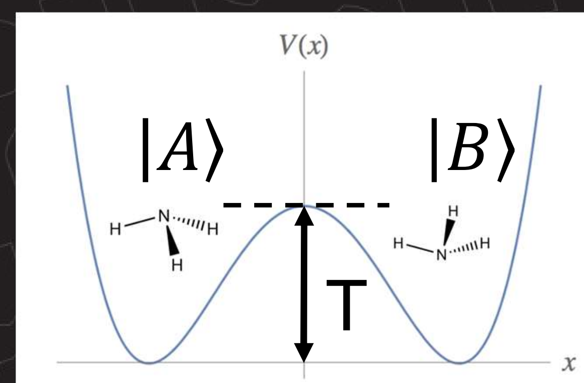
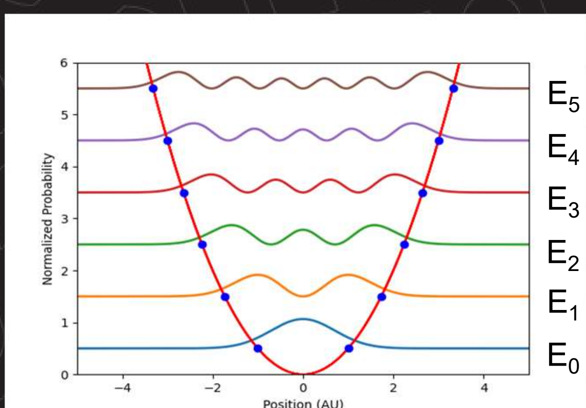
Ursinus College Physics Department





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What is Quantum Chemistry?

- Quantum chemistry (QC) is a branch of chemistry that sits on the boundary between quantum mechanics and physical chemistry.
- The goal of QC is to determine the chemical and physical properties of a molecule or material through quantum mechanical calculations.

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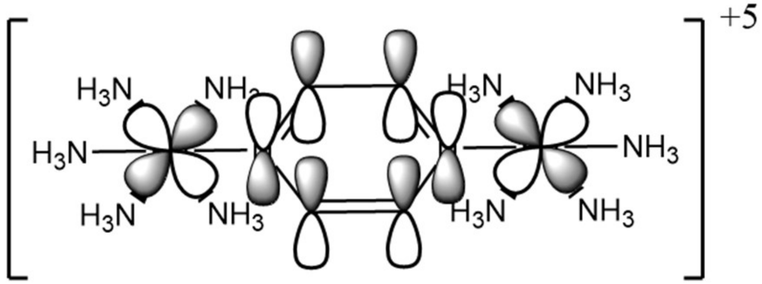
Why Does This Matter?

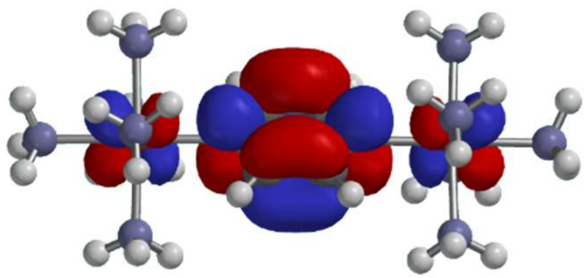
- Quantum chemistry allows chemists to do theoretically any experiment they could desire.
- Months in a lab could be whittled down to just hours with parallel computations.
- Spending on solvents, reagents, and standards could be cut by a large percentage.

Practical Application

Predicted



Computer Verified



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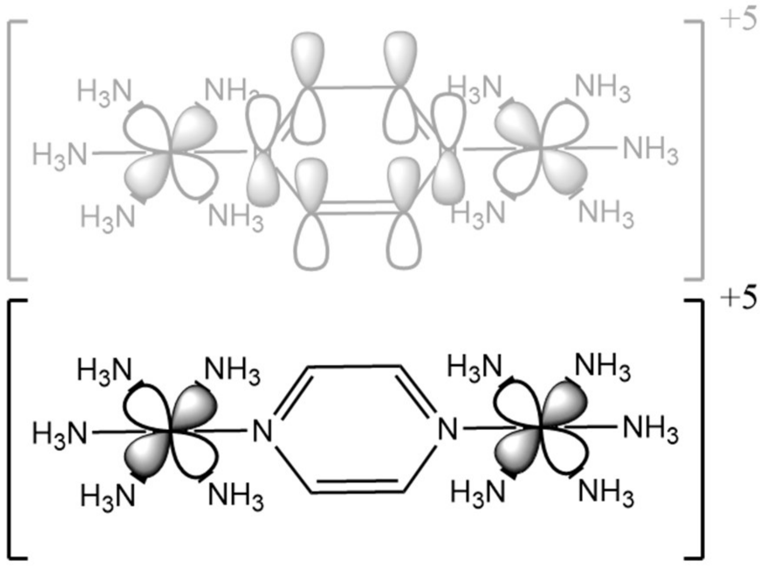
Practical Application

Predicted



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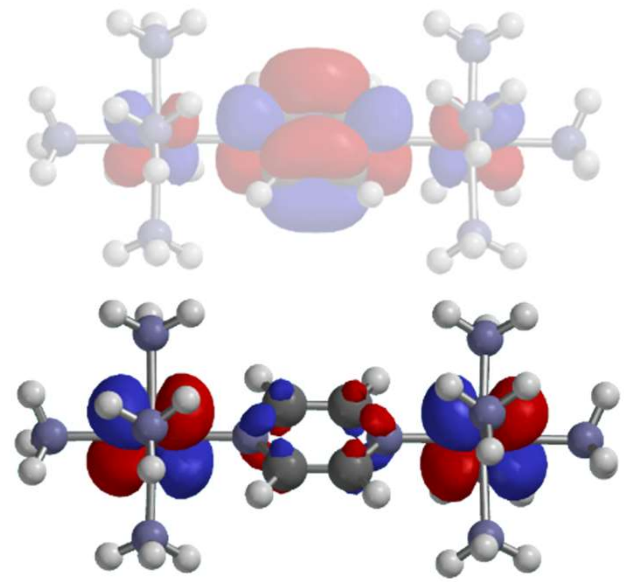
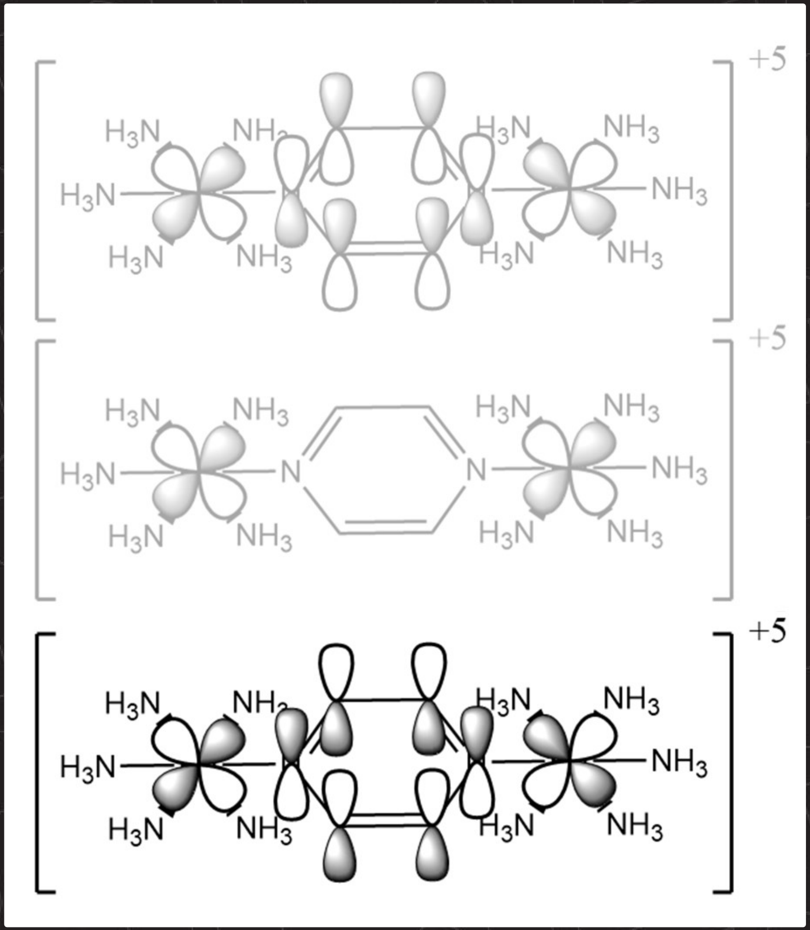


Practical Application

Predicted



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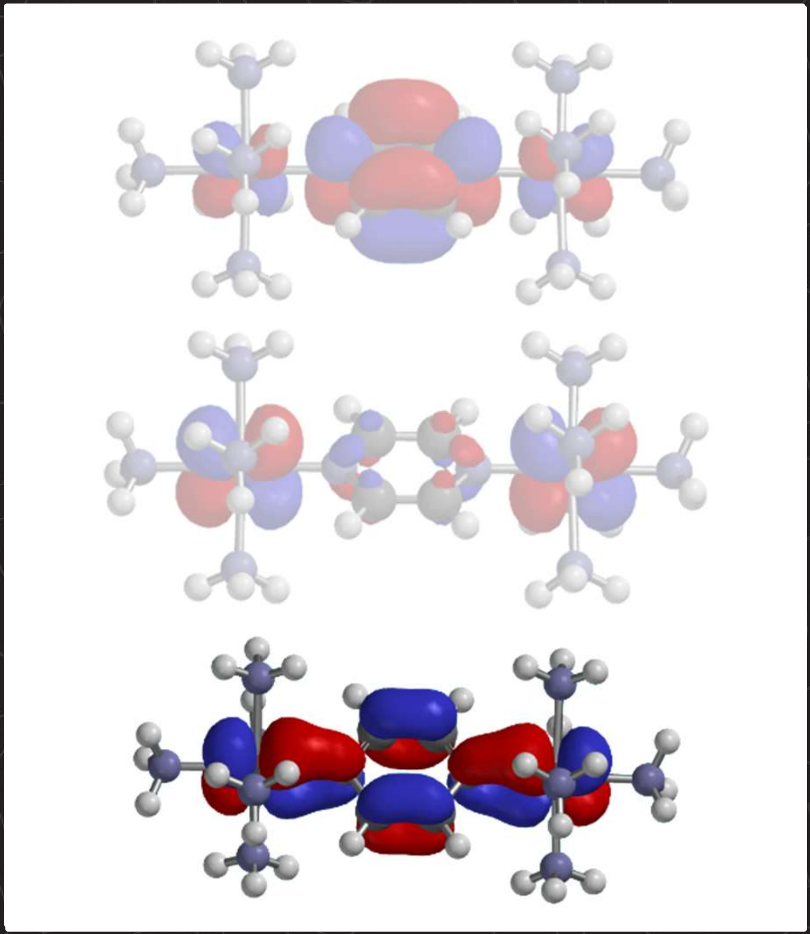

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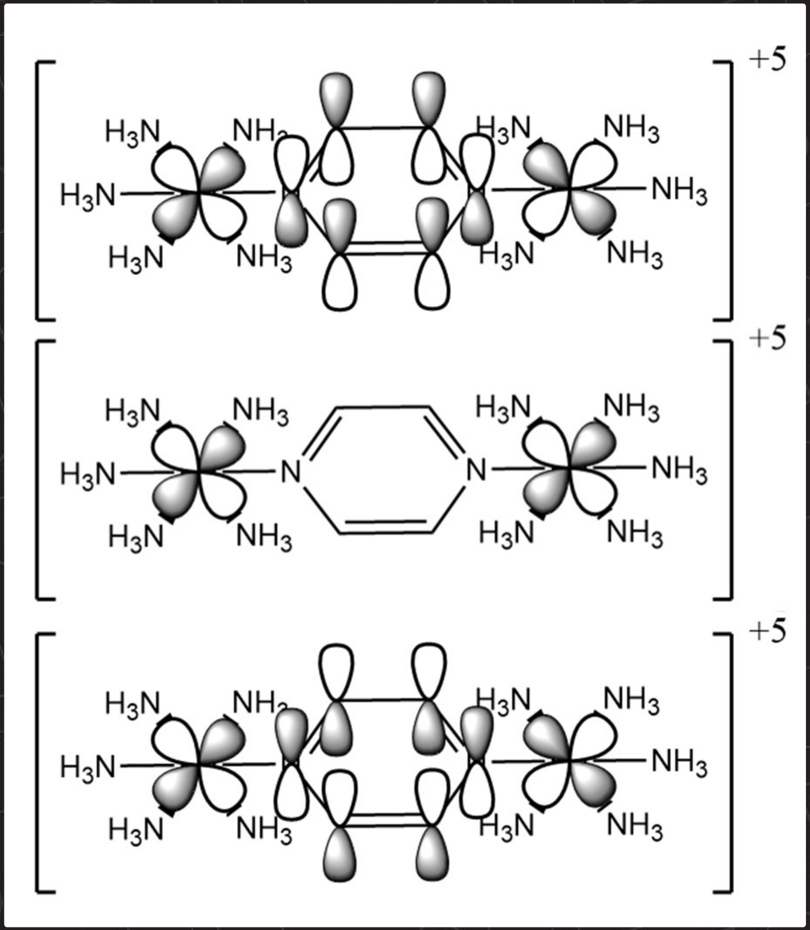
Practical Application

Predicted



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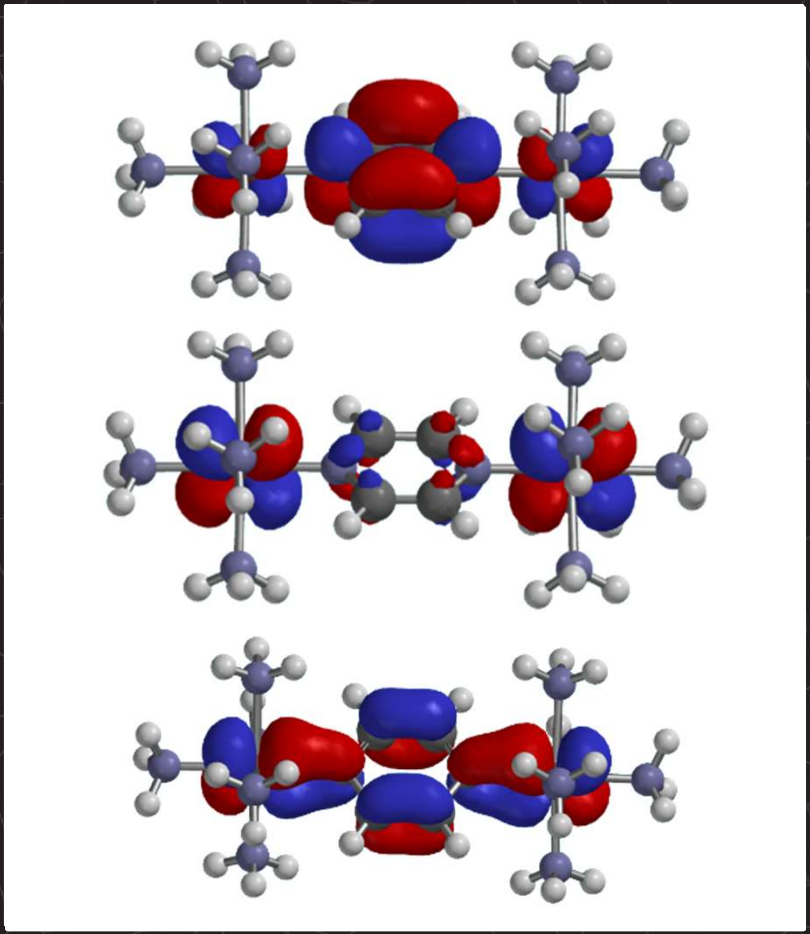

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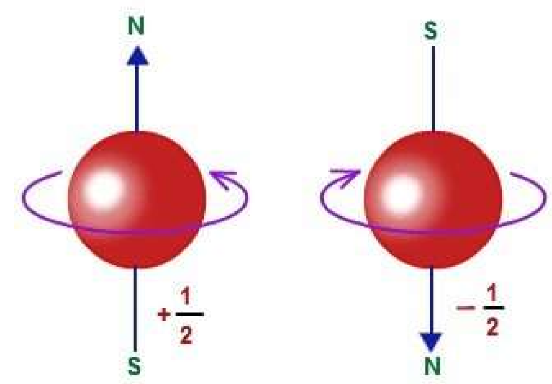
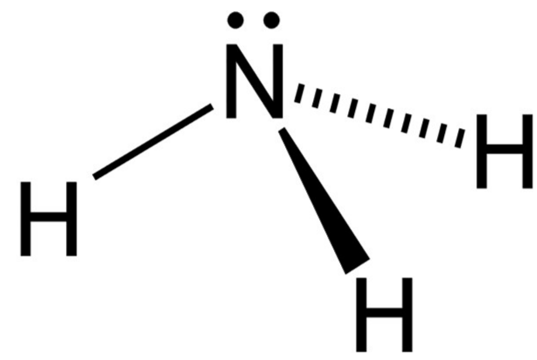
Outline of Progress

1. Study of quantum spin states
   1. Spin operators
   2. Eigenvalues and Eigenvectors
2. Time evolution of particles
   1. Time evolution operator
   2. Energy Operator
   3. Magnetic Resonance
3. Ammonia Masers
   1. Two-state quantum system
   2. Tunneling
   3. Energy eigenstates
4. Python Programming
   1. Harmonic Oscillator
   2. First Program





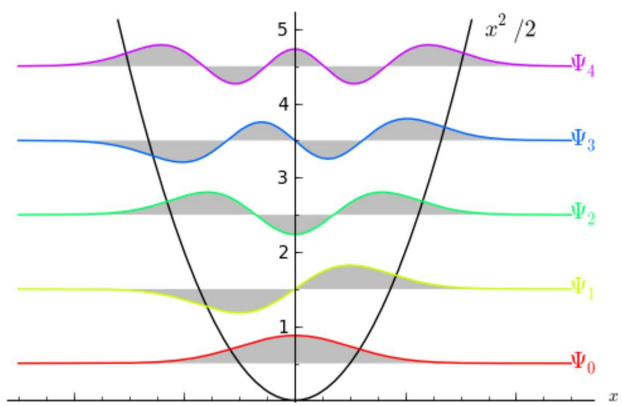


Image sources (top to bottom)
https://www.quantum-field-theory.net/discovery-electron-spin/
https://www.acs.org/molecule-of-the-week/archive/a/ammonia.html
https://owlcation.com/stem/schrodinger-equation-simple-harmonic-oscillator

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Quantum Spin States

- Almost every particle in the universe has an intrinsic spin
- Spin states are the direct cause of several fundamental aspects of nature, such as orbitals, Pauli exclusion, and at a macroscopic scale, magnetism.
- All spin states are represented by operators, typically denoted $\hat{S}$ (read as "S hat"), that describe the spin of a particle.

$$\hat{S}_x \underset{z}{\rightarrow} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

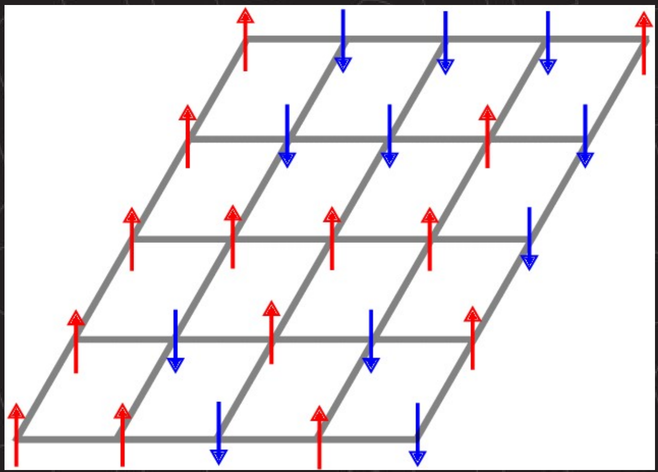
$$\hat{S}_y \underset{z}{\rightarrow} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\hat{S}_z \underset{z}{\rightarrow} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\hat{S}_x \underset{z}{\rightarrow} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

$$\hat{S}_y \underset{z}{\rightarrow} \begin{pmatrix} 0 & i & 0 \\ -i & 0 & i \\ 0 & -i & 0 \end{pmatrix}$$

$$\hat{S}_z \underset{z}{\rightarrow} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$



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Surprise Linear Algebra!

- A critical component of operator matrices are the associated eigenvalues and eigenvectors.
- The eigenvalue problem is primarily a linear algebra topic, and I had to learn it to continue.
- An understanding of linear algebra gives critical insight into how computers process quantum mechanical inputs

$$\hat{H}|\psi\rangle = E|\psi\rangle$$

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \times \begin{bmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \end{bmatrix}$$

$$= \begin{bmatrix} a_{11}b_{11}+a_{12}b_{21}+a_{13}b_{31} & a_{11}b_{12}+a_{12}b_{22}+a_{13}b_{32} & a_{11}b_{13}+a_{12}b_{23}+a_{13}b_{33} \\ a_{21}b_{11}+a_{22}b_{21}+a_{23}b_{31} & a_{21}b_{12}+a_{22}b_{22}+a_{23}b_{32} & a_{21}b_{13}+a_{22}b_{23}+a_{23}b_{33} \\ a_{31}b_{11}+a_{32}b_{21}+a_{33}b_{31} & a_{31}b_{12}+a_{32}b_{22}+a_{33}b_{32} & a_{31}b_{13}+a_{32}b_{23}+a_{33}b_{33} \end{bmatrix}$$

Image Source: https://www.mymathtables.com/calculator/matrix/3-cross-3-matrix-multiplication.html

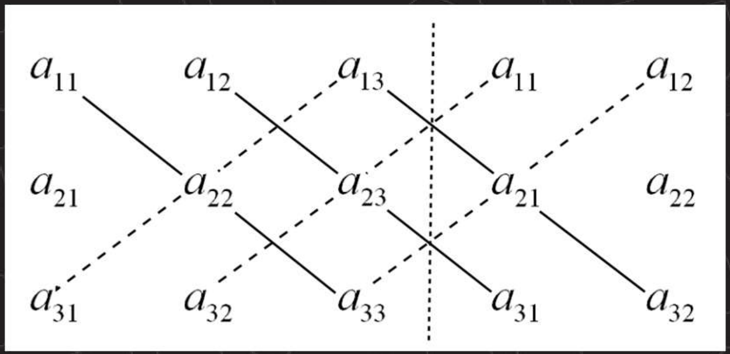

Image Source: Wikimedia Commons

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Time Evolution of Quantum Systems

- The time evolution operator, $\hat{U}(t)$ is used to determine how a system behaves over time.
- Time is what gives everything meaning, if the universe was locked at one time, it would be worthless.
- The operator, at infinitesimal increment, can be described with the "generator of time evolutions"

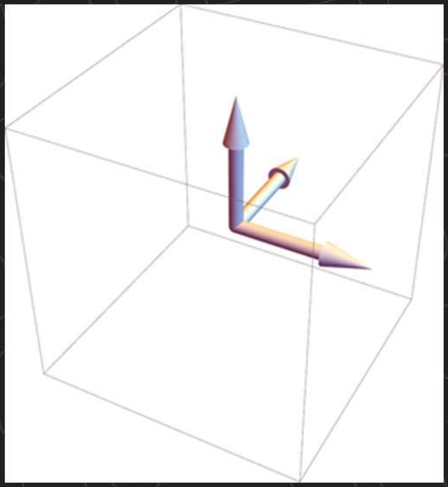

Image Source: https://www.joerg-enderlein.de/dzhanibekov

$$\hat{U}(dt) = 1 - \frac{i}{\hbar}\hat{H}dt$$

$$\hat{U}^{\dagger}(dt) = 1 + \frac{i}{\hbar}\hat{H}^{\dagger}dt$$

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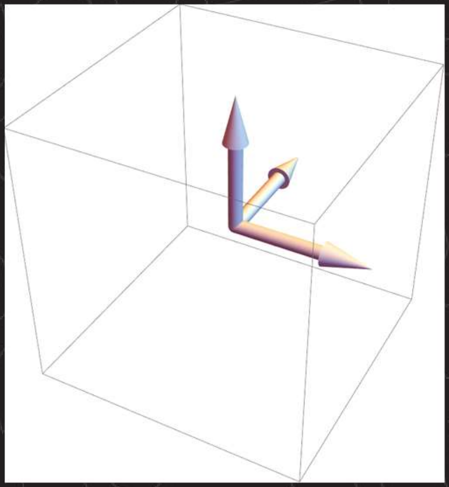

Image Source: https://www.joerg-enderlein.de/dzhanibekov

$$\hat{U}(dt) = 1 - \frac{i}{\hbar}\hat{H}dt$$

$$\hat{U}^{\dagger}(dt) = 1 + \frac{i}{\hbar}\hat{H}^{\dagger}dt$$

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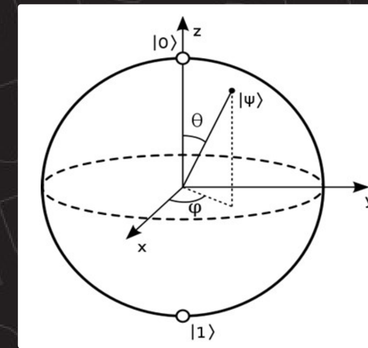
Energy Operator

- The energy operator, also known as the Hamiltonian is denoted as $\hat{H}$ and is king of operators
- The Hamiltonian takes in a wavefunction and returns the energy of it at a specific time.
- This operator plays a critical role in quantum chemistry

$$\hat{H} = \frac{-gq}{2mc}\hat{S} \cdot (B_1 \cos(\omega t)\, i + B_0 k)$$

$$\begin{pmatrix} E_0 & -T \\ -T & E_0 \end{pmatrix} \begin{pmatrix} \langle 1|\psi\rangle \\ \langle 2|\psi\rangle \end{pmatrix} = E \begin{pmatrix} \langle 1|\psi\rangle \\ \langle 2|\psi\rangle \end{pmatrix}$$

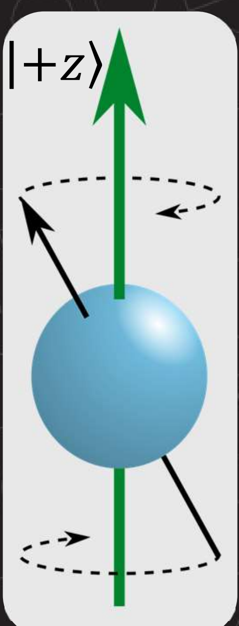
Image Source:
Wikimedia Commons



Magnetic Resonance

- Magnetic resonance is a consequence of intrinsic spin, as all particles with spin have a magnetic field around them.

$$|\langle -z|\psi(t)\rangle|^2 = \sin^2\frac{\omega_1 t}{4} \qquad |\langle +z|\psi(t)\rangle|^2 = \cos^2\frac{\omega_1 t}{4}$$



$$|\langle -z|\psi(t)\rangle|^2 = \frac{\omega_1^2/4}{(\omega_0-\omega)^2+\omega_1^2/4}\sin^2\frac{t}{2}\sqrt{(\omega_0-\omega)^2+\omega_1^2/4}$$

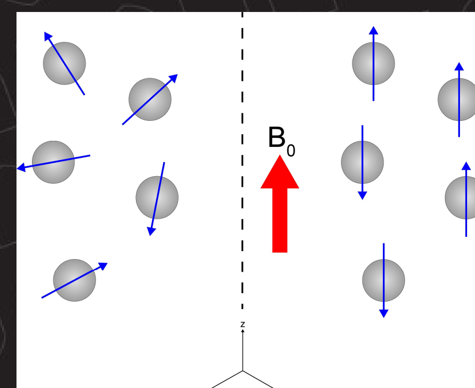


Image Source:
https://maxfacts.uk/diagnosis/tests/mri/detailed

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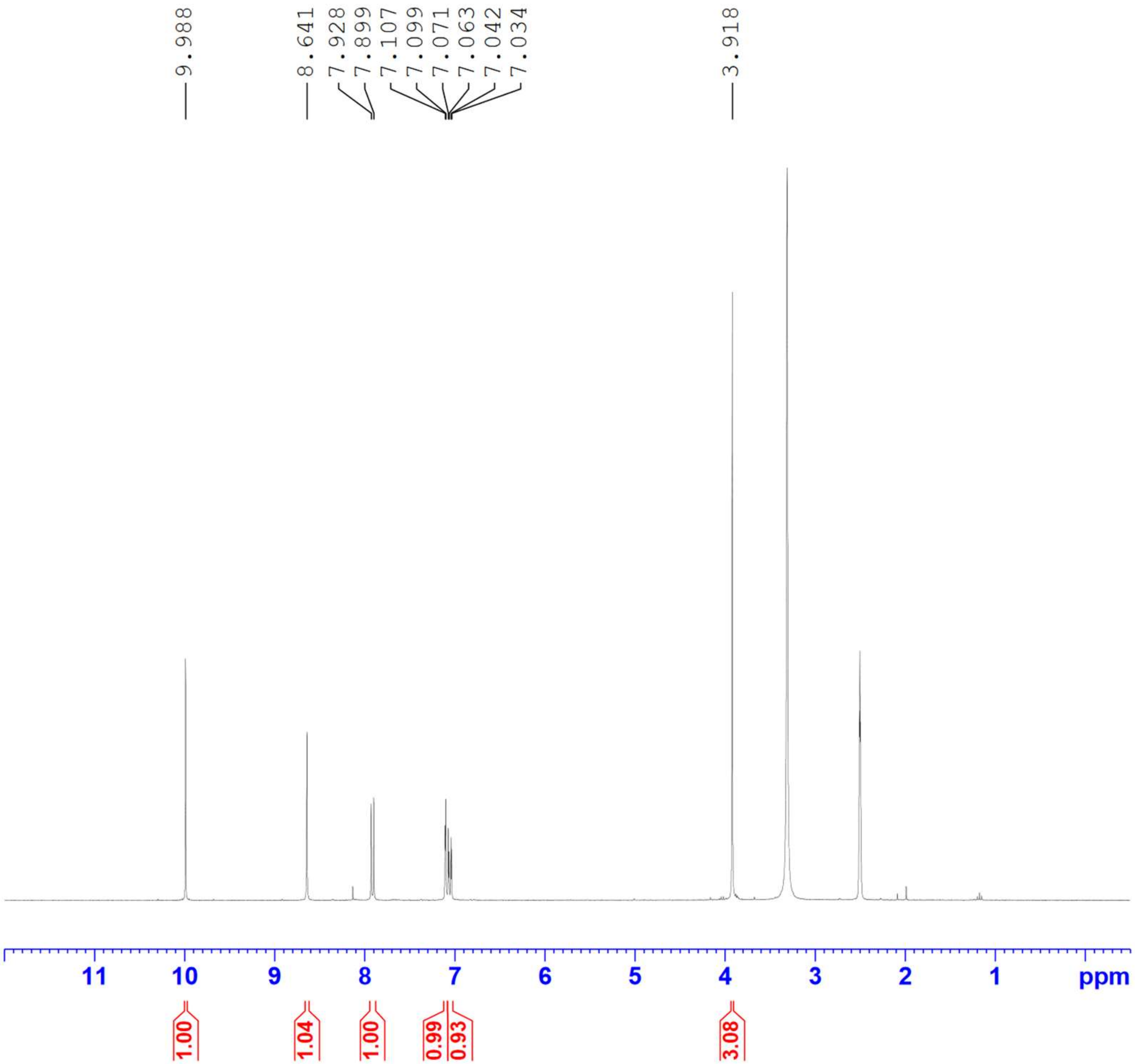
Image Source:
Wikimedia Commons

Image Source: Bruker Ascend NMRs



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PROCNO                 1

F2 - Acquisition Parameters
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Time               16.16 h
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PROBHD    Z104275_0403 (
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                   128
DS                     2
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ             5.4525952 sec
RG                208.95
DW                83.200 usec
DE                  6.50 usec
TE                 300.0 K
D1            1.00000000 sec
TD0                    1
SFO1         300.1318533 MHz
NUC1                  1H
P1                 14.00 usec
PLW1          7.85349989 W

F2 - Processing parameters
SI                 65536
SF           300.1300026 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

Ammonia Masers

- A common example of a two-state quantum system is the ammonia maser, first proposed by Richard Feynman in the 1960s.
- The system is also backed by real experimental data from labs that commonly use ammonia to mase.

$$\hat{H} \rightarrow \begin{pmatrix} \langle A|\hat{H}|A\rangle & \langle A|\hat{H}|B\rangle \\ \langle B|\hat{H}|A\rangle & \langle B|\hat{H}|B\rangle \end{pmatrix} \rightarrow \begin{pmatrix} E_0 & -T \\ -T & E_0 \end{pmatrix}$$

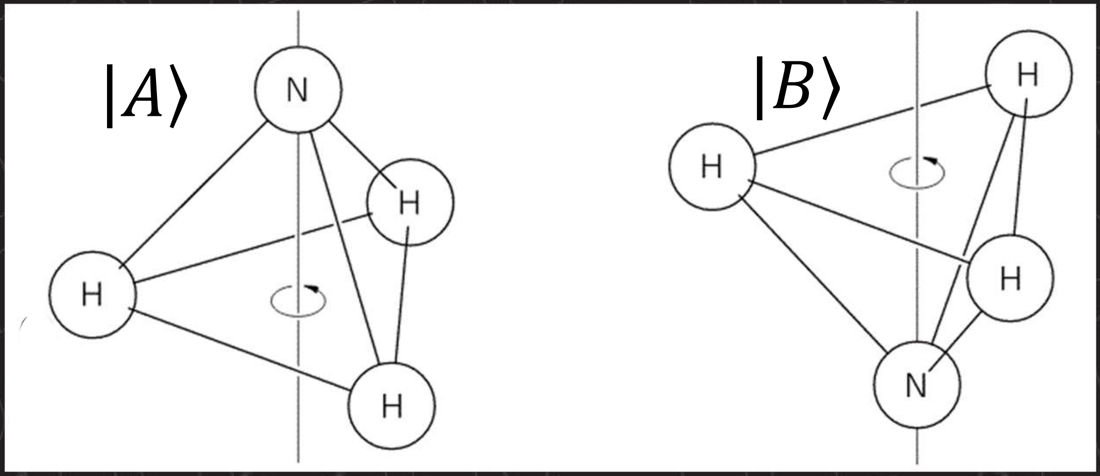
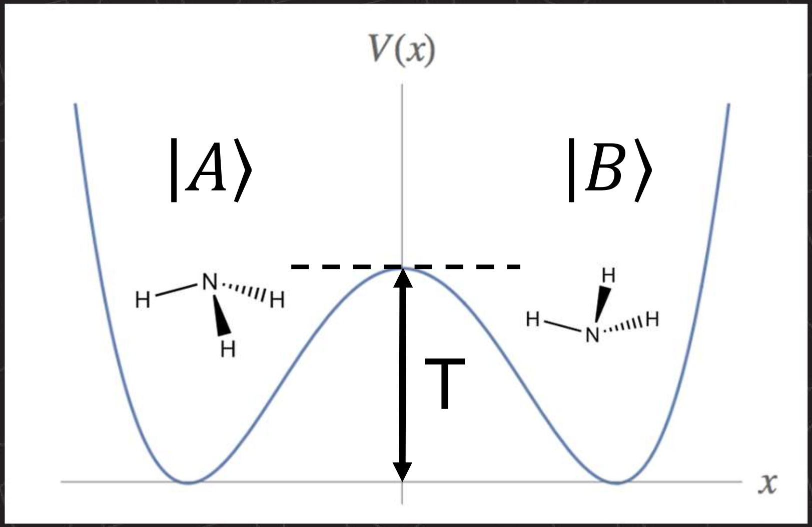


Image Source: https://readingfeynman.org/2015/12/01/the-math-behind-the-maser-re-visited/

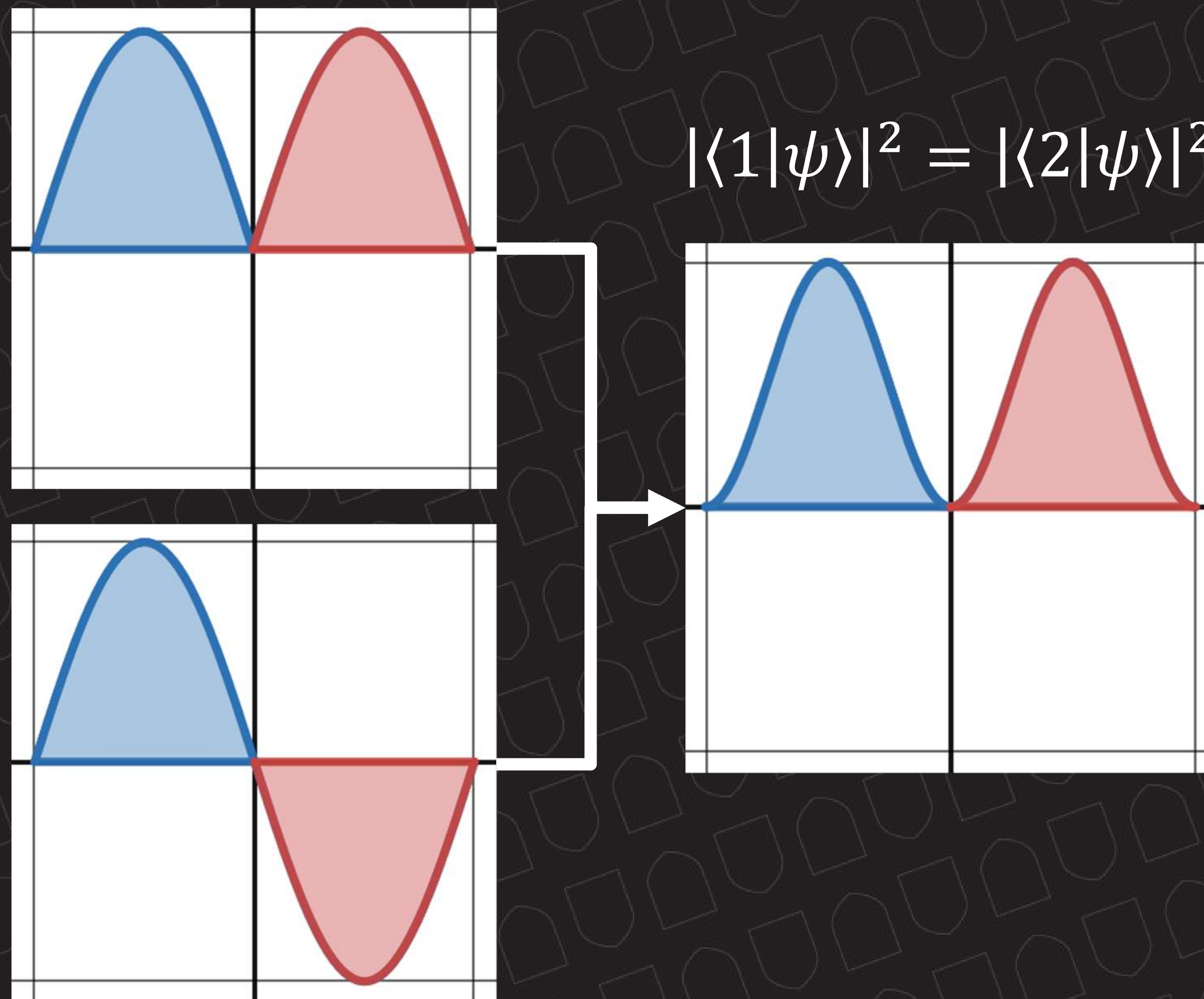


Graph From: “Ammonia Inversion Energy Levels using Operator Algebra” by S.M. Blinder

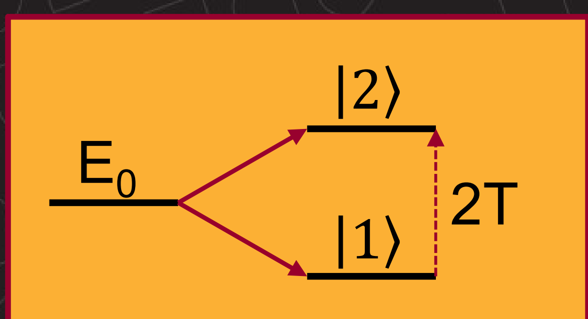
Non-Degenerate States

$$|1\rangle = \frac{1}{\sqrt{2}}|A\rangle + \frac{1}{\sqrt{2}}|B\rangle$$

$$|2\rangle = \frac{1}{\sqrt{2}}|A\rangle - \frac{1}{\sqrt{2}}|B\rangle$$



$$|\langle 1|\psi\rangle|^2 = |\langle 2|\psi\rangle|^2$$



The Quantum Harmonic Oscillator

- An exact solvable model for harmonic systems, such as atoms in an optical lattice or in a diatomic molecule.
- It approximates potential energy as a parabola and shows the probability of finding a molecule in a specific position in that well.

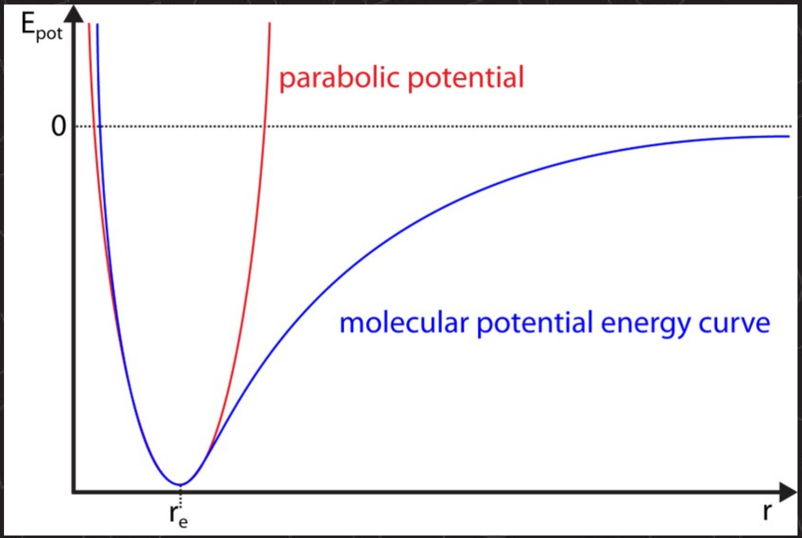
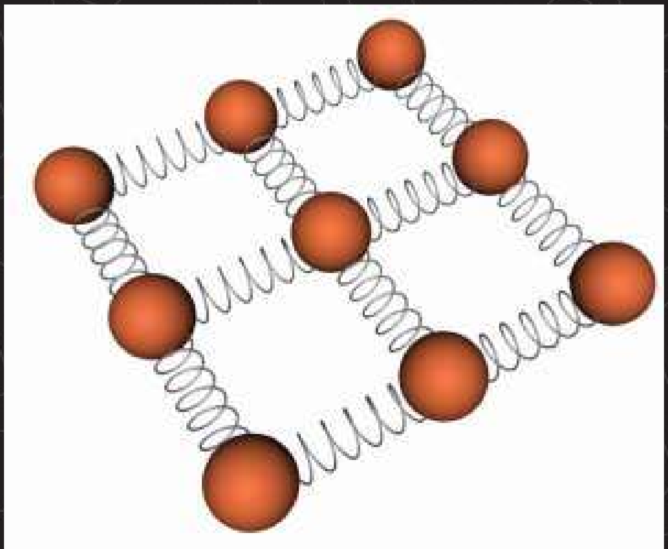


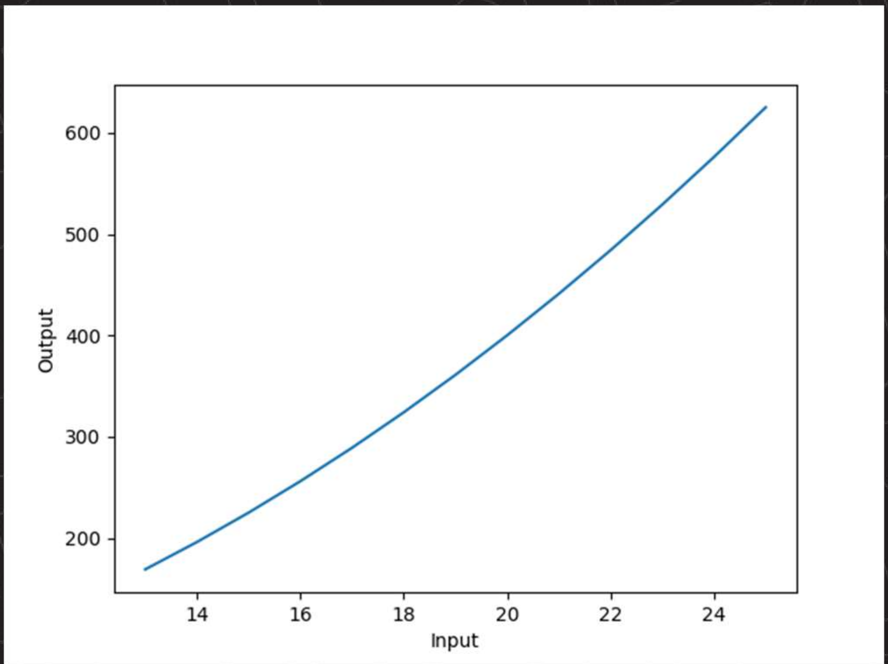
Image Credit: David Degler, ResearchGate.net



Programming in Python

- A critical component of this research is computer programming, of which I had little to no experience
- To learn Python, I made several programs to gain an adequate grasp on the fundamentals.

```python
import numpy as np
import matplotlib.pyplot as plt
import scipy as sp
import sys
import os.path
x = int(input("Min value: "))
y = int(input("Max value: "))
input_list = np.arange(x, y+1)
output_list = []
combined_list = []
for i in range(x, y+1):
    square = i**2
    print(i, "-->", square)
    output_list.append(square)
plt.plot(input_list, output_list)
plt.xlabel("Input")
plt.ylabel("Output")
plt.savefig(image_path)
plt.show()
```



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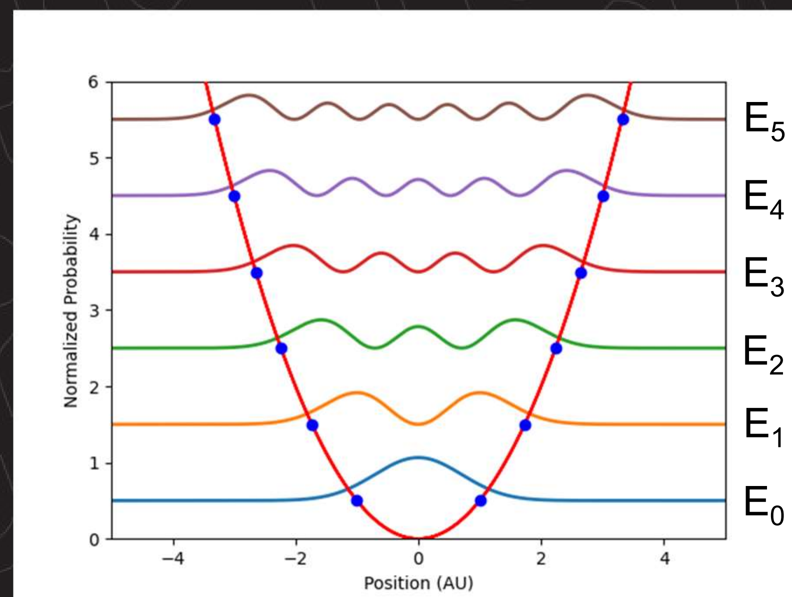
```
initial = [((alpha / pi) ** (1/4)) * sy.exp((-m * w * (x**2))/(2 * hbar))]

def derivative(x, intFunction):
    df = sy.diff(intFunction, x)
    return df


for i in n:
    raised = (1/math.sqrt(i+1)) * (sy.sqrt(alpha/2)) * ((x * initial[i]) - (derivative(x, initial[i])))
    initial.append(raised)

x_range = np.arange(-5, 5, 0.01)
y_range = np.arange(0, choice, 1)

plt.figure()
plt.xlim([-5,5])
plt.ylim([-0,choice])
for r in n:
    plot = sy.lambdify(x, initial[r]**2+(r+0.5))
    n_turnpoint = -math.sqrt(2*y_range[i]+1)
    p_turnpoint = math.sqrt(2*y_range[i]+1)
    plt.plot(x_range, plot(x_range), linewidth=2, zorder=2)
    #plt.axvline(x = -math.sqrt(2*y_range[r] + 1), linestyle='dashed', color='#5f5dff', zorder=1)
    #plt.axvline(x = math.sqrt(2*y_range[r] + 1), linestyle='dashed', color='#5f5dff', zorder=1)
    plt.plot(x_range, (x_range**2/2), linestyle='-', color='r', zorder=3)
    plt.plot(-math.sqrt(2*y_range[r] + 1), y_range[r]+0.5, 'o', color='b', zorder=4)
    plt.plot(math.sqrt(2*y_range[r] + 1), y_range[r]+0.5, 'o', color='b', zorder=4)
plt.show()
```



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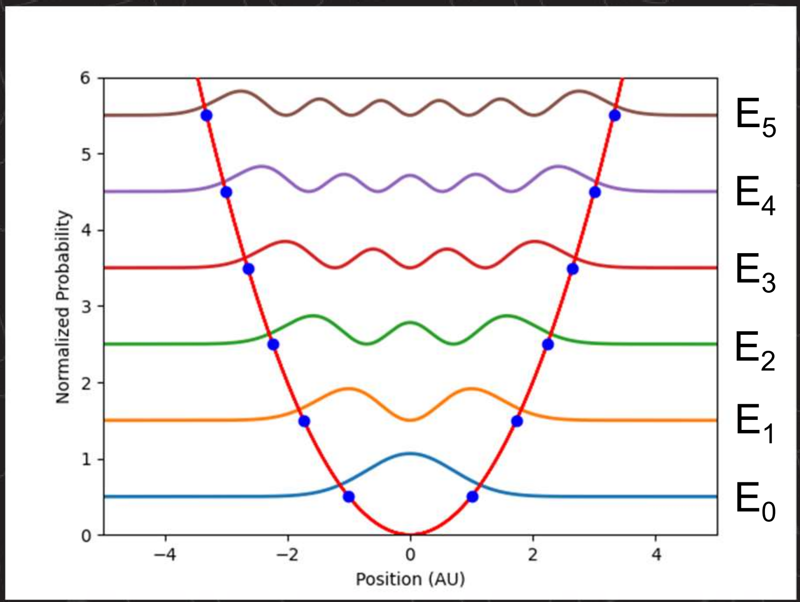
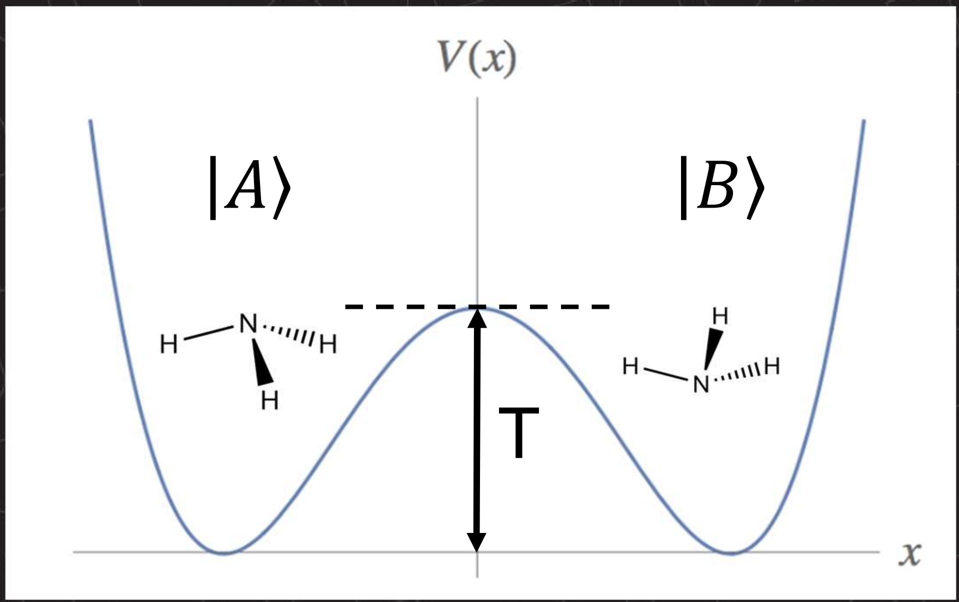
Next Steps





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Acknowledgements

- Ursinus College
- UC Physics and Chemistry Departments
- Summer Fellows Coordinators
- Dylan Ford and Ryan R. Walvoord for NMR Data
- Ross B. Martin-Wells
- John and Dona Dyer

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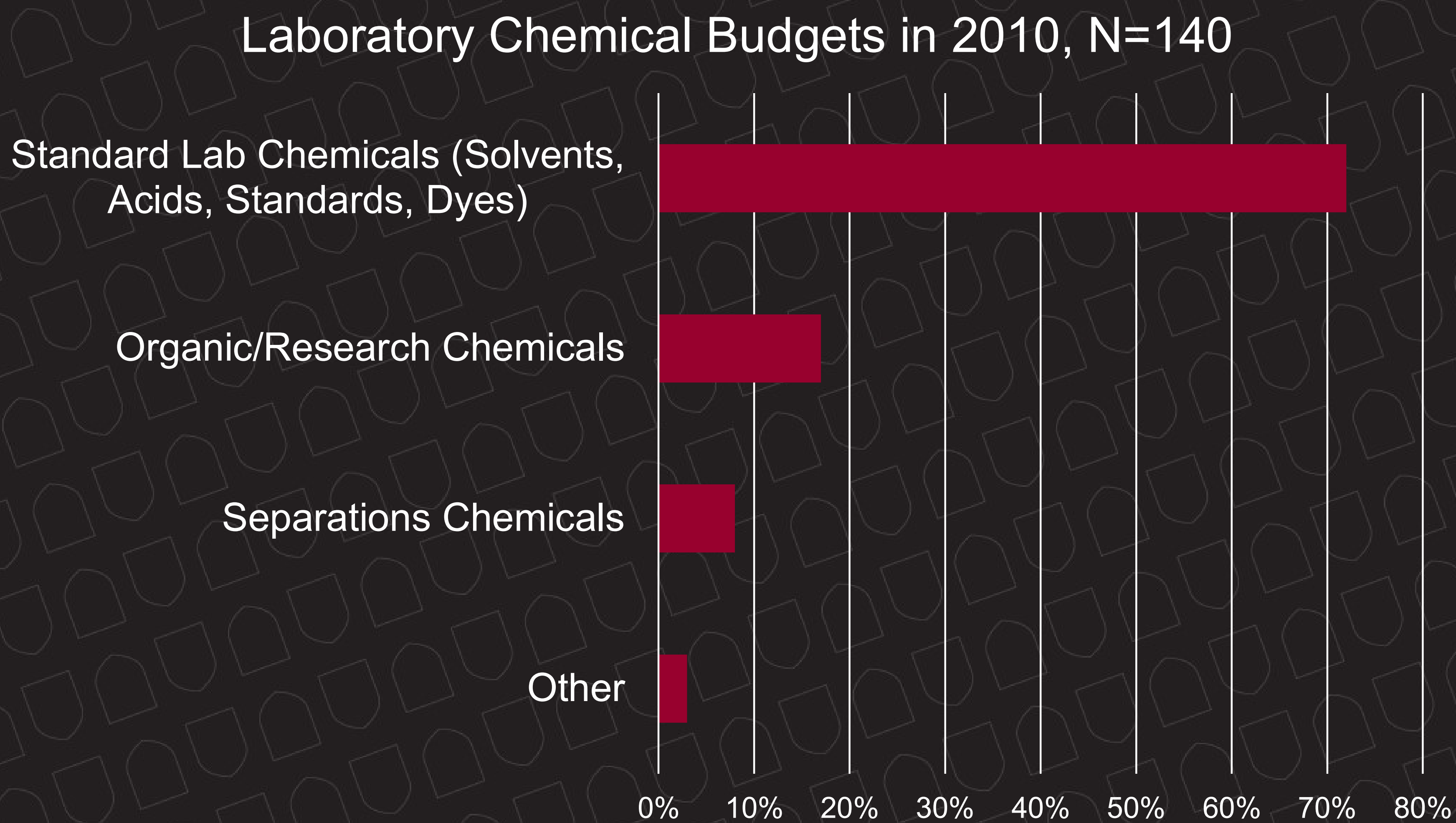
Lab Chemical Spending

Average Spending across all labs is $48,400



Source: Frost & Sullivan analysis.

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