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### Enhanced Quantum Chemistry With Machine Learning

Brock Dyer Ursinus College, brdyer@ursinus.edu

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## Enhanced Quantum Chemistry with Machine Learning.

Brock Dyer, Chemistry and Physics Major, Class of 2025 Professor Ross B. Martin-Wells Ursinus College Physics Department  $V(x)$ 





## What is Quantum Chemistry?

- wat is Quantum Chemistry?<br>• Quantum chemistry (QC) is a branch of<br>• Chemistry that sits on the boundary between chemistry that sits on the boundary between quantum mechanics and physical chemistry. what is Quantum Chemistry?<br>• Quantum chemistry (QC) is a branch of<br>• chemistry that sits on the boundary between<br>• The goal of QC is to determine the chemical<br>• The goal of QC is to determine the chemical<br>• and physical pr
- and physical properties of a molecule or material through quantum mechanical calculations.



## Why Does This Matter?

- Thy Does This Matter?<br>• Quantum chemistry allows chemists to do<br>• doctrolly any experiment they could theoretically any experiment they could desire. we provide the Matter of the Matter of the Matter of the theoretically any experiment they could desire.<br>
• Months in a lab could be whittled down to just<br>
hours with parallel computations. • Quantum chemistry allows chemists to do<br>theoretically any experiment they could<br>desire.<br>• Months in a lab could be whittled down to ju<br>hours with parallel computations.<br>• Spending on solvents, reagents, and<br>standards cou
- hours with parallel computations.
- standards could be cut by a large percentage.



# Practical Application Tactical Application







# Practical Application **Predicted Computer Verified Computer Veri**





# Practical Application **Predicted Computer Verified Computer Veri**





# Practical Application Tactical Application





## Outline of Progress Utline of Progress 1. Spin operators<br>
1. Spin operators<br>
2. Eigenvalues and Eigenvectors<br>
1. Spin operators<br>
1. Spin operators<br>
1. Spin operators<br>
Time evolution of particles Utline of Progress<br>
1. Study of quantum spin states<br>
1. Spin operators<br>
2. Eigenvalues and Eigenvectors<br>
2. Time evolution of particles<br>
1. Time evolution operator<br>
2. Energy Operator 1. Time **of Progress**<br>
1. Spin operators<br>
2. Eigenvalues and Eigenvectors<br>
1. Time evolution of particles<br>
1. Time evolution operator<br>
2. Energy Operator<br>
3. Magnetic Resonance **1. IIME Of Progress**<br>
2. Eigenvalues and Eigenvectors<br>
2. Eigenvalues and Eigenvectors<br>
2. Eigenvalues and Eigenvectors<br>
1. Time evolution operator<br>
2. Energy Operator<br>
3. Magnetic Resonance<br>
Ammonia Masers **Solution Study of quantum spin states<br>
3. Spin operators<br>
2. Eigenvalues and Eigenvectors<br>
2. Eigenvalues and Eigenvectors<br>
1. Time evolution operator<br>
2. Energy Operator<br>
3. Magnetic Resonance<br>
Ammonia Masers<br>
1. Two-sta** 1. Study of quantum spin states<br>
1. Spin operators<br>
2. Eigenvalues and Eigenvectors<br>
2. Time evolution of particles<br>
1. Time evolution operator<br>
2. Energy Operator<br>
3. Magnetic Resonance<br>
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1. Two-state qu

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





### Quantum Spin States

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

$$
\hat{S}_x \rightarrow \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \hat{S}_x \rightarrow \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}
$$
  
\n
$$
\hat{S}_y \rightarrow \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \hat{S}_y \rightarrow \begin{pmatrix} 0 & i & 0 \\ -i & 0 & i \\ 0 & -i & 0 \end{pmatrix}
$$
  
\n
$$
\hat{S}_z \rightarrow \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad \hat{S}_z \rightarrow \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}
$$



### Surprise Linear Algebra!

- First Component of operator matrices are the<br>
A critical component of operator matrices are the<br>
associated eigenvalues and eigenvectors. associated eigenvalues and eigenvectors.
- First Contract and the eigenvalue problem is primarily a linear algebra.<br>
 A critical component of operator matrices are the<br>
 The eigenvalue problem is primarily a linear algebra<br>
 An understanding of linear algebra gi topic, and I had to learn it to continue.
- valid of the University of the Cassociated eigenvalues and eigenvectors.<br>
 A critical component of operator matrices are the<br>
 The eigenvalue problem is primarily a linear algebra<br>
 An understanding of linear algebra gi insight into how computers process quantum mechanical inputs

### $\widehat{H}|\psi\rangle = E|\psi\rangle$

 $=$ 



 $a_{11}b_{11} + a_{12}b_{21} + a_{13}b_{31}$   $a_{11}b_{12} + a_{12}b_{22} + a_{13}b_{32}$   $a_{11}b_{13} + a_{12}b_{23} + a_{13}b_{33}$  $a_{21}b_{11} + a_{22}b_{21} + a_{23}b_{31}$   $a_{21}b_{12} + a_{22}b_{22} + a_{23}b_{32}$   $a_{21}b_{13} + a_{22}b_{23} + a_{23}b_{33}$  $a_{31}b_{11} + a_{32}b_{21} + a_{33}b_{31}$   $a_{31}b_{12} + a_{32}b_{22} + a_{33}b_{32}$   $a_{31}b_{13} + a_{32}b_{23} + a_{33}b_{33}$ 





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Image Source: Wikimedia Commons

## Time Evolution of Quantum Systems me Evolution of Quantum<br>
ystems<br>
• The time evolution operator,  $\hat{U}(t)$  is used to<br>
determine how a system behaves over time. **Find the Find of Quantum**<br> **vstems**<br>
• The time evolution operator,  $\bar{U}(t)$  is used to<br>
• Time is what gives everything meaning, if the<br>
• Time is what gives everything meaning, if the<br>
worthless.

- determine how a system behaves over time.
- universe was locked at one time, it would be worthless. vertical intervalses and the evolution of the time evolution operator,  $\hat{U}(t)$  is used to determine how a system behaves over time.<br>
• Time is what gives everything meaning, if the universe was locked at one time, it wo
- described with the "generator of time evolutions" In the operator, at infinitesides<br>
In the "gene  $\widehat{U}(dt)$ <br>
In the system of the

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

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



## Time Evolution of Quantum Systems me Evolution of Quantum<br>
ystems<br>
• The time evolution operator,  $\hat{U}(t)$  is used to<br>
determine how a system behaves over time. **Find the Find of Quantum**<br> **vstems**<br>
• The time evolution operator,  $\bar{U}(t)$  is used to<br>
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- determine how a system behaves over time.
- universe was locked at one time, it would be worthless. vertical intervalses and the evolution of the time evolution operator,  $\hat{U}(t)$  is used to determine how a system behaves over time.<br>
• Time is what gives everything meaning, if the universe was locked at one time, it wo
- described with the "generator of time evolutions" The operator, at infinitesi<br>described with the "gene $\widehat{U}(dt)$





## Energy Operator

- ergy Operator<br>• The energy operator, also known as the Hamiltonian<br>• The Hamiltonian takes in a wavefunction and returns is denoted as  $\widehat{H}$  and is king of operators • The energy operator, also known as the Hamiltonian<br>
is denoted as  $\hat{H}$  and is king of operators<br>
• The Hamiltonian takes in a wavefunction and returns<br>
the energy of it at a specific time.<br>
• This operator plays a cr
- **Paramer of the Hamiltonian Control of the Hamiltonian**<br>• The energy operator, also known as the Hamiltonian<br>• The Hamiltonian takes in a wavefunction and returns<br>• This energy of it at a specific time. the energy of it at a specific time.
- chemistry





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

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## Magnetic Resonance



agnetic Resonance is a consequence of intrinsic<br>
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Priv spin, as all particles with spin have a magnetic field around them.

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

 $2 \pm 74$  $1/\gamma$  $27700077$  $0 - \omega$ )<sup>-</sup> + -  $\frac{1}{4}$  $2 + \frac{\omega_1}{\omega_1}$   $\sim$   $\sim$   $\sim$   $\sim$ 2,  $311\overline{2} \sqrt{60}$   $\omega$  $2 \frac{1}{2} \left[ \frac{1}{(a)} (a) \right]^{2} + \frac{\omega_1}{2}$  $0 \top \omega$ <sup>-+</sup>  $\uparrow \wedge$ 4 )  $\smile$  $2 + \frac{\omega_1}{\sqrt{2}}$  $2 \times 11$ 



miage Source:<br>Wikimedia Commons<br>Wikimedia Commons



### Ammonia Masers

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

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

![](_page_16_Figure_4.jpeg)

![](_page_16_Picture_5.jpeg)

![](_page_16_Figure_6.jpeg)

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

![](_page_16_Picture_8.jpeg)

![](_page_17_Figure_0.jpeg)

## The Quantum Harmonic **Oscillator**

- **1e Quantum Harmonic<br>
Scillator<br>
 An exact solvable model for harmonic systems, such<br>
as atoms in an optical lattice or in a diatomic<br>
molecule** as atoms in an optical lattice or in a diatomic molecule. • Quantum Harmonic<br>
• An exact solvable model for harmonic systems, such<br>
as atoms in an optical lattice or in a diatomic<br>
molecule.<br>
• It approximates potential energy as a parabola and<br>
shows the probability of finding a
- shows the probability of finding a molecule in a specific position in that well.

![](_page_18_Figure_3.jpeg)

![](_page_18_Picture_4.jpeg)

## Programming in Python

- Formal Component of this research is computer<br>
To loarn Python I had little to no experience programming, of which I had little to no experience
- For a continuing the analysis of the several program of this research is computer.<br>
 A critical component of this research is computer.<br>
 To learn Python, I made several programs to gain an<br>
 adequate grasp on the funda adequate grasp on the fundamentals.

```
\Boximport 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 = []\Box for i in range(x, y+1):
     square = i**2print(i, "--"), square)
     output_list.append(square)
 plt.plot(input_list, output_list)
 plt.xlabel("Input")
 plt.ylabel("Output")
 plt.savefig(image_path)
 plt.show()
```
![](_page_19_Figure_4.jpeg)

## Programming in Python

Formal component of this research is computer<br>
To loarn Python I had little to no experience programming, of which I had little to no experience

For a continuing the analysis of the several program of this research is computer.<br>
• A critical component of this research is computer.<br>
• To learn Python, I made several programs to gain an<br>
• adequate grasp on the funda adequate grasp on the fundamentals.

```
initial = [((\alpha \ln x) * (1/4)) * (1/4)) * (1/4) * (1/4) * (1/4) * (1/4) * (1/4) * (1/4) * (1/4) * (1/4) * (1/4) * (1/4) * (1/4) * (1/4) * (1/4) * (1/4) * (1/4) * (1/4) * (1/4) * (1/4) * (1/4) * (1/4) * (1/4) * (1/4) * (1/4) * (1/4) * (1/4) * (1/4) * (1/4) * (1/4) * (1/4) * (1/4) * (1/4) * (1/
```

```
\existsdef derivative(x, intFunction):
     df = sy.diff(intFunction, x)return df
```
### $\Box$ for i in n:

```
raised = (1/math.sqrt(i+1)) * (sy.sqrt(abha/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])
\existsfor r in n:
     plot = sy.lambdify(x, initial[r]**2+(r+0.5))
     n_tturnpoint = -math.sqrt(2*y_t)range[i]+1)
     p_{\text{}}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()
```
![](_page_20_Figure_10.jpeg)

## Next Steps

![](_page_21_Figure_1.jpeg)

![](_page_21_Figure_2.jpeg)

## **Acknowledgements** CKnowledgements<br>• Ursinus College<br>• UC Physics and Chemistry De **EXHOWLedgements<br>• University Departments<br>• UC Physics and Chemistry Departments<br>• Summer Fellows Coordinators** Cknowledgements<br>• Ursinus College<br>• UC Physics and Chemistry Departments<br>• Summer Fellows Coordinators<br>• Dylan Ford and Ryan R. Walvoord for NMR **Example Concerned School Schools**<br>• UC Physics and Chemistry Depart<br>• Summer Fellows Coordinators<br>• Dylan Ford and Ryan R. Walvoord<br>• Ross B. Martin-Wells<br>• John and Dona Dyer

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- **Exhowledgements<br>• Ursinus College<br>• UC Physics and Chemistry Departments<br>• Dylan Ford and Ryan R. Walvoord for NMR Data<br>• Ross B. Martin-Wells** • Ursinus College<br>• UC Physics and Chemistry Depar<br>• Summer Fellows Coordinators<br>• Dylan Ford and Ryan R. Walvoord<br>• Ross B. Martin-Wells<br>• John and Dona Dyer
- 
- 

![](_page_22_Picture_7.jpeg)

## Lab Chemical Spending

Laboratory Chemical Budgets in 2010, N=140 Average Spending across all labs is \$48,400

Standard Lab Chemicals (Solvents, Acids, Standards, Dyes)

Organic/Research Chemicals

Separations Chemicals

**Other** 

0% 10% 20% 30% 40% 50% 60% 70% 80%