

Quantum Mechanics: A Pedagogical Approach to a Geometric Theory

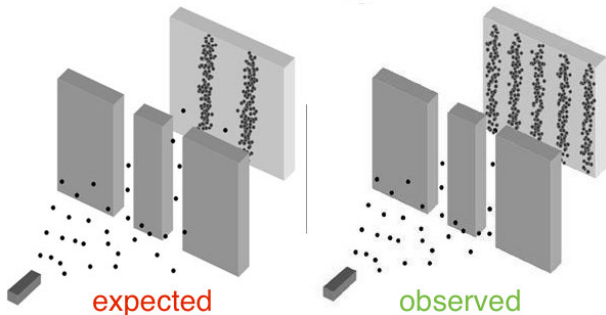
Guilherme Dias Vianna

Dead Physicists Society

The Wall

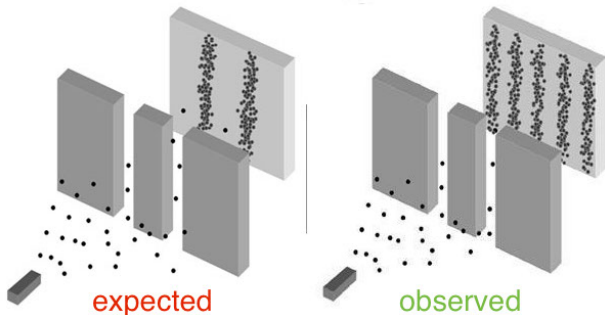
One big failure

- Double Slit Experiment:



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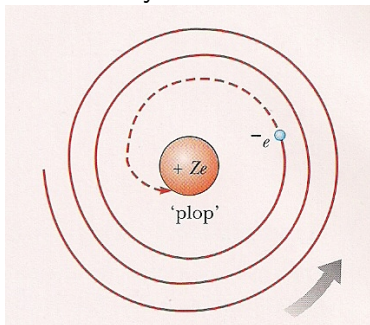
- Double Slit Experiment:



- Particles behave like waves? Superposition effects??

Ok, now that's bad

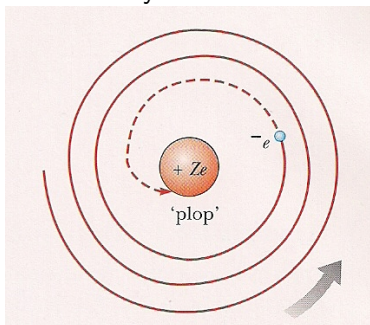
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- According to Larmor's formula $\left(P = \frac{q^2 a^2}{6\pi\epsilon_0 c^3} \right)$
- How come matter is stable?

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 - Most physical quantities (energy, for instance) take discrete values in the atomic scale!
 - When we measure our system, it seems that we interfere with it!
 - Only certain "configurations" seem right!

Quantum Mechanics!

Each more beautiful than the last!

First Postulate:

All the information of a physical system (or, more precisely, it's **state**) is represented by a **vector** $|\phi\rangle$ in a given **Hilbert space** \mathcal{H} .

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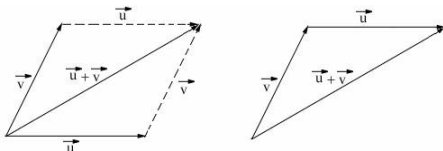
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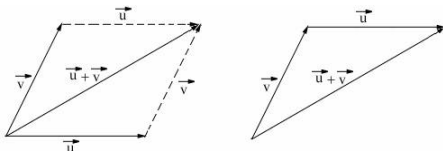
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$$\vec{u} + \vec{v} \longrightarrow |\mathbf{u}\rangle + |\mathbf{v}\rangle$$

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A small detour in eigenproblems

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If the dimension is **infinite**, we need to solve a **differential equation!**

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EXPONENTIAL OF A MATRIX??

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$$e^{\hat{A}} = \mathbb{1} + \hat{A} + \frac{1}{2}\hat{A}^2 \dots$$

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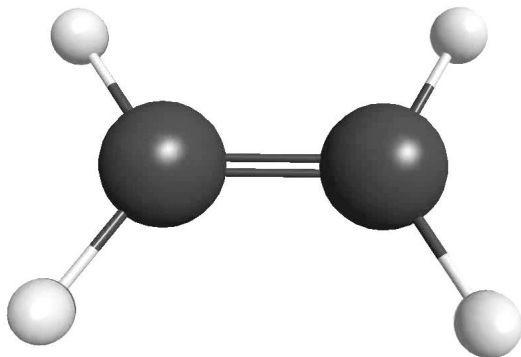
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- Hermitian operators always have **real** eigenvalues!

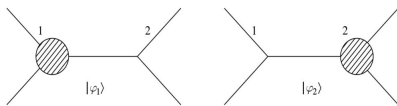
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- The use of vectors and complex numbers guarantees superposition!
- Hermitian operators always have **real** eigenvalues!
- The use of scalar products guarantees that the usual probability laws hold just fine!

The Ethylene Molecule

1530 cm^{-1}





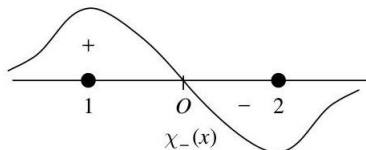
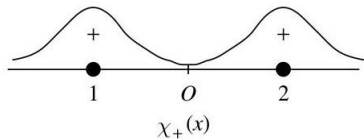
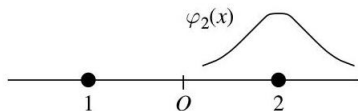
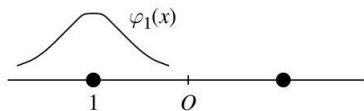
The most general hamiltonian in this case is:

$$\hat{\mathcal{H}} = \begin{pmatrix} E_0 & -A \\ -A & E_0 \end{pmatrix}$$

It's eigenvalues/vectors are:

$$E_{\pm} = E_0 \mp A, |\chi_{\pm}\rangle = \frac{1}{\sqrt{2}}(|\phi_1\rangle \pm |\phi_2\rangle)$$

By projecting $|\chi_{\pm}\rangle$ onto the basis of position $|x\rangle$ (more to come about this):



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Reason: Since there are a continuous number of "wanted eigenvalues" and the domain of this operator is not quite clear, this operator is **unbounded** in \mathcal{H} ! (so $|\mathbf{x}\rangle$ are not really elements of \mathcal{H} , even though they form a of basis!)

The third and final detour

In reality, $|\mathbf{x}\rangle$ are elements of the space of tempered **distributions** \mathcal{D}' ! It can be shown that $\mathcal{H} \subset \mathcal{D}'$

They form a basis in the a sense and are subject to the relation:

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Improper normalization!

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If we project a state vector $|\psi(t)\rangle$ onto this subspace we get something called a **wavefunction**!

$$\langle \mathbf{x} | \psi \rangle = \psi(\mathbf{x}, t)$$

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We get it on the representation of space:

$$i\hbar\frac{\partial\psi}{\partial t}(\mathbf{x}, t) = \mathcal{H}\psi(\mathbf{x}, t)$$

A partial differential equation!

What have you brought upon this cursed land...

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Where $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ is called the laplacian operator

In the case of the hydrogen atom:

$$V(r) = -\frac{1}{4\pi\epsilon_0} \frac{e^2}{r}$$

The eigenvalue problem

I could try to walk you through the resolution of what's left

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$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \varphi^2}$$

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- Then we would need to solve the eigenvalue problem:

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + -\frac{1}{4\pi\epsilon_0} \frac{e^2}{r} \right) \psi = E\psi$$

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- We can use the separation of variables (because that's God's command):

$$\psi(r, \theta, \varphi) = R(r)\Theta(\theta)\Phi(\varphi)$$

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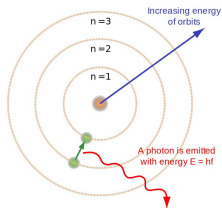
Quantum Numbers			Eigenfunctions
n	l	m_l	
1	0	0	$\psi_{100} = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$
2	0	0	$\psi_{200} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \left(2 - \frac{Zr}{a_0}\right) e^{-Zr/2a_0}$
2	1	0	$\psi_{210} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \frac{Zr}{a_0} e^{-Zr/2a_0} \cos \theta$
2	1	± 1	$\psi_{21\pm 1} = \frac{1}{8\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \frac{Zr}{a_0} e^{-Zr/2a_0} \sin \theta e^{\pm i\varphi}$
3	0	0	$\psi_{300} = \frac{1}{81\sqrt{3\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \left(27 - 18\frac{Zr}{a_0} + 2\frac{Z^2 r^2}{a_0^2}\right) e^{-Zr/3a_0}$
3	1	0	$\psi_{310} = \frac{\sqrt{2}}{81\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \left(6 - \frac{Zr}{a_0}\right) \frac{Zr}{a_0} e^{-Zr/3a_0} \cos \theta$
3	1	± 1	$\psi_{31\pm 1} = \frac{1}{81\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \left(6 - \frac{Zr}{a_0}\right) \frac{Zr}{a_0} e^{-Zr/3a_0} \sin \theta e^{\pm i\varphi}$

And does it work?

This solutions gives us:

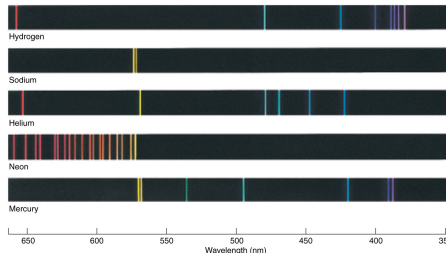
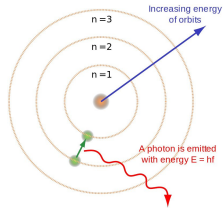
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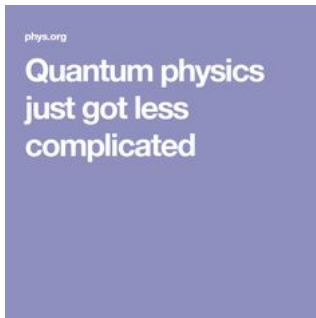


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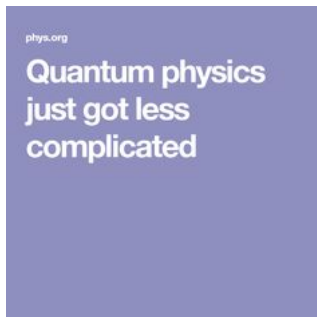
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Thank you!