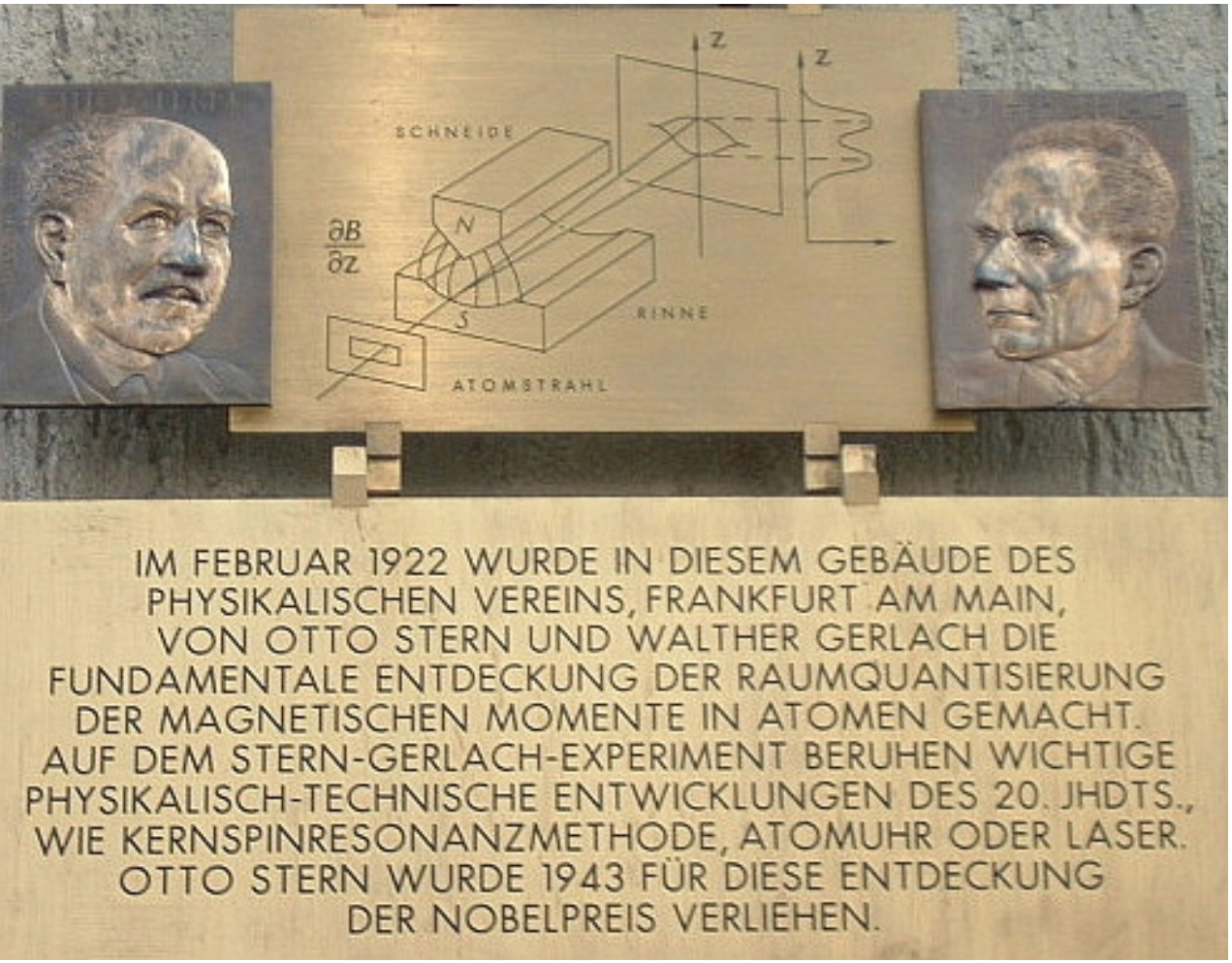
An Important 2-State System: Spin 1/2



Stern-Gerlach Experiment

Energy of magnet in a magnetic field

$$U = -\boldsymbol{\mu} \cdot \mathbf{B}$$

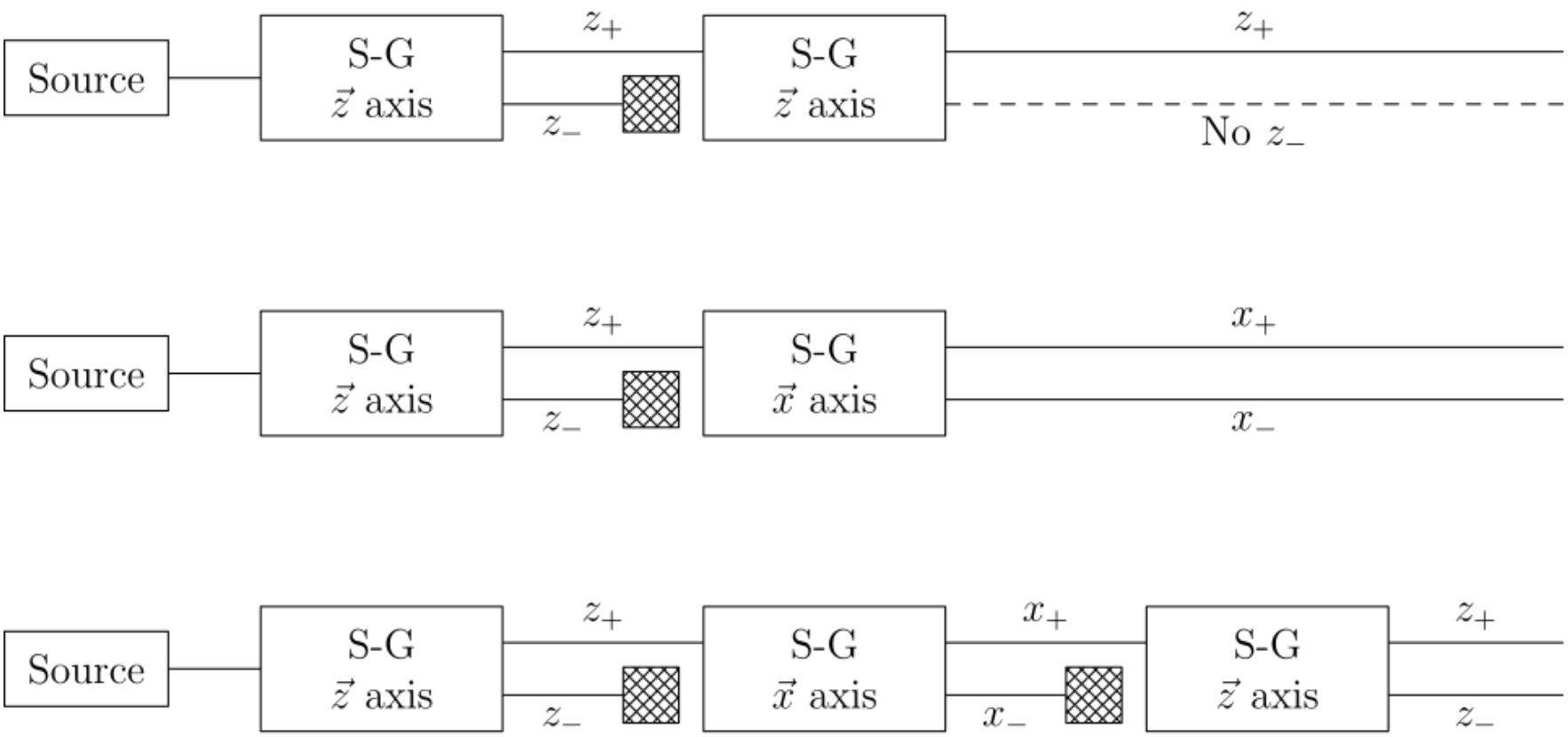
Force on the magnet

$$F = -\frac{\partial U}{\partial z} = -\boldsymbol{\mu} \cdot \frac{\partial \mathbf{B}}{\partial x}$$

Particles deflection determined by μ_z. In other words, the S-G apparatus measures μ_z.

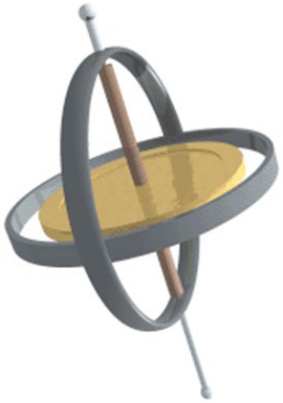
Watch the animation at http://en.wikipedia.org/wiki/Stern%E2%80%93Gerlach_experiment

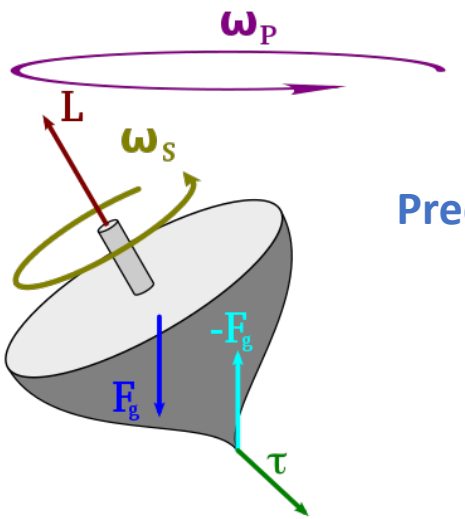
Sequential Stern-Gerlach (S-G) experiments



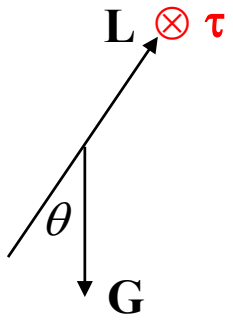
https://en.wikipedia.org/wiki/Stern%E2%80%93Gerlach_experiment

To understand the electron and other quantum spins, let's first look at classical ones – spinning tops





Precession



Watch animation at
https://en.wikipedia.org/wiki/Top

https://en.wikipedia.org/wiki/Angular_momentum

Point mass motion analogy	Rigid body rotation
$\mathbf{p} = m\mathbf{v}$	$\mathbf{L} = I\boldsymbol{\omega}$
	moment of inertia
$\mathbf{F} = d\mathbf{p}/dt$	$\boldsymbol{\tau} = d\mathbf{L}/dt$

Let the distance from spinning top centroid-to-tip distance be l. The torque is $\tau = lF_g \sin\theta$.

$$dL/dt = \omega_p L \sin\theta$$

$$\Rightarrow \quad \omega_p = \tau/(L\sin\theta) = lF_g/L = lF_g/(I\omega)$$

The factor lF_g/I is determined by the top's geometry.

$$\omega_p \propto 1/\omega$$

Exercise: A spinning top's mass is concentrated in ring of radius R, centered at distance l from the tip. The angular momentum is $L = mRv = mR^2\omega$. Using $F_g = mg$, show that $\omega_p = g(l/R^2)/\omega$.

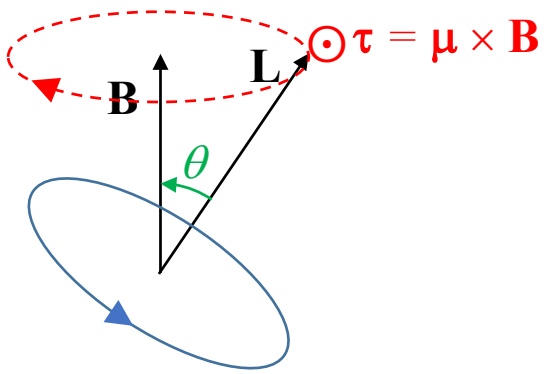
Now, our spinning top is a point charge Q orbiting along a circle of radius R, at a constant angular speed ω, in a **B** field; no gravity.

$$L = mRv = mR^2\omega$$

current

The magnetic moment $\mu = \pi R^2(Q\omega/2\pi) = (Q/2)R^2\omega = (Q/2m)(mR^2\omega) = (Q/2m)L.$

$$\boldsymbol{\mu} = (Q/2m)\mathbf{L}$$



$\boldsymbol{\mu}$ // **L**, proportional constant is $Q/2m$.

$\boldsymbol{\tau} = \boldsymbol{\mu} \times \mathbf{B}$ $\qquad\qquad$ $\tau = (Q/2m)LB\sin\theta$

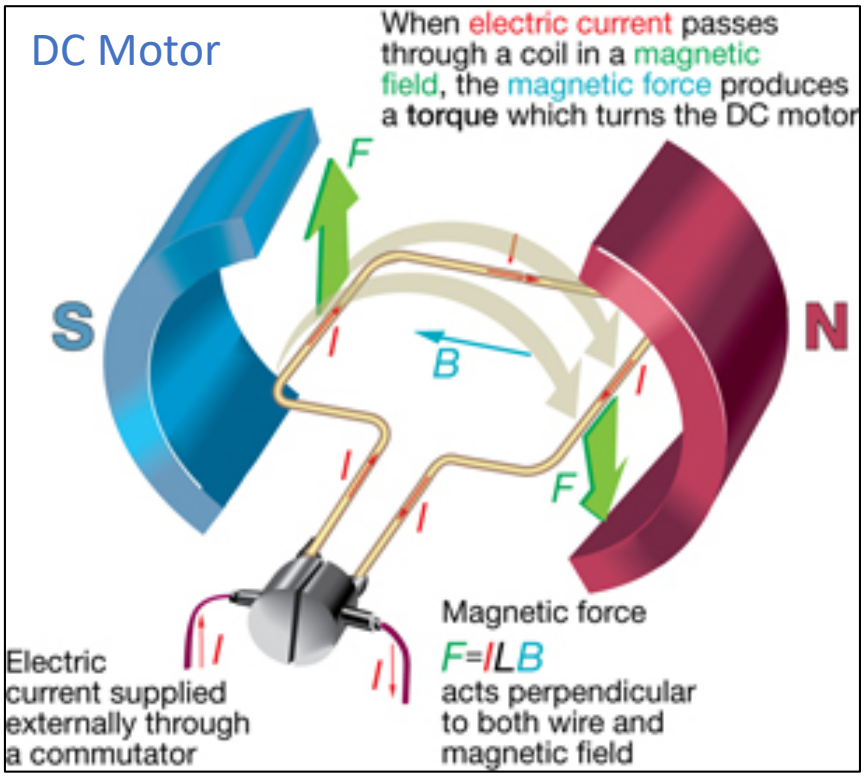
Notice that $\tau \propto L$ here, unlike the gravitation case.

$$\omega_p = \tau/(L\sin\theta) = (Q/2m)B$$

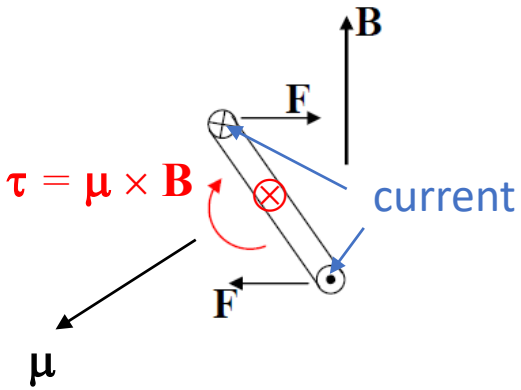
ω_p depends only on the properties of the particle and the field B.

Without external disturbance, the field **B** cannot change the projection of **L** (or, concomitantly, $\boldsymbol{\mu}$) onto the direction of **B**, i.e., $\boldsymbol{\mu}\cdot\mathbf{B}$ is constant.
L (or $\boldsymbol{\mu}$) precedes around **B**.
The field **B** does not align **L** (or $\boldsymbol{\mu}$) to itself.

The free orbiter is very different from the axis-fixed coil in a motor, which would eventually align to **B** if the electrical brush was not used.



http://resource.rockyview.ab.ca/rvlc/physics30_BU/Unit_B/m4/p30_m4_l03_p4.html



Why?

The coil, as a rigid body, has no angular momentum if not driven by the magnetic field.

For the orbiter, having an angular momentum in the absence of the magnetic field, the torque exerted by the field is "used" to steer the angular momentum.

A turning wheel does not fall, as all bicyclists know.

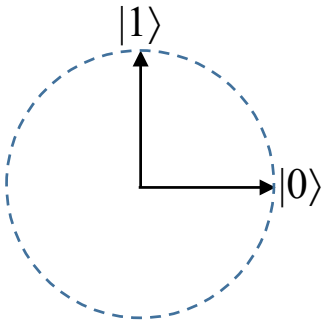
Quantum mechanics interpretation of the S-G experiment

Spin angular momentum **S** is intrinsic to the electron. The associated magnetic momentum $\boldsymbol{\mu} \propto -\mathbf{S}$.

The S-G apparatus measures the projection of **S** in a direction, say the z axis. There can only be two outcomes, $+\hbar/2$ and $-\hbar/2$. These are called the two eigenvalues. Each of them corresponds to an eigenstate.

The two states are regarded two orthogonal vectors, labeled $|\uparrow\rangle$ and $|\downarrow\rangle$ in Dirac notation. Or, we may label them $|0\rangle$ and $|1\rangle$ in the context of quantum computing.

The electron's spin state is described by $|\chi\rangle = c_\uparrow|\uparrow\rangle + c_\downarrow|\downarrow\rangle$, where $c_\uparrow$ and $c_\downarrow$ are complex numbers, satisfying $|c_\uparrow|^2 + |c_\downarrow|^2 = 1$. We just say that $|\uparrow\rangle$ and $|\downarrow\rangle$ form an orthonormal basis set. The electron spin is a 2-state system. Any possible spin state is in the 2D space defined by $|\uparrow\rangle$ and $|\downarrow\rangle$. Therefore, $|\uparrow\rangle$ and $|\downarrow\rangle$ form a complete basis.



Not exactly representing A spin state, since the amplitudes are in general complex.
(not to be confused with the Bloch Sphere)

In the basis of $|\uparrow\rangle$ and $|\downarrow\rangle$ (or $|0\rangle$ and $|1\rangle$),

$$|\uparrow\rangle = |0\rangle = \begin{pmatrix}1\\0\end{pmatrix}, \quad |\downarrow\rangle = |1\rangle = \begin{pmatrix}0\\1\end{pmatrix}, \quad \text{and } |\chi\rangle = \begin{pmatrix}c_\uparrow\\c_\downarrow\end{pmatrix}.$$

An electron spin is a qubit. This is how a qubit is different from a classical bit:
The states of a classical bit can only be two points is the 2D state space.
The states of a qubit are richer than the blue dashed circle, since the amplitudes are complex (phase matters).

$|c_\uparrow|^2$ and $|c_\downarrow|^2$ are the probabilities of finding the electron in $|\uparrow\rangle$ and $|\downarrow\rangle$, respectively.

A measurement of a physical quantity only results in eigenvalues.
That is, any arbitrary state of a quantum system "collapse" to an eigenstate upon measurement.
A physical quantity is represented by an operator, which is a matrix in the state space.

Say, a physical quantity is represented by an operator **Q**, the eigenvalues are $q_0, q_1, \ldots, q_n, \ldots$, corresponding to eigenstates $|0\rangle, |1\rangle, \ldots, |n\rangle, \ldots$, then $\mathbf{Q}|n\rangle = q_n|n\rangle$.

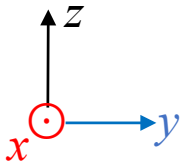
Confused? The simple 2-state spin make it easy to understand.

Here, the physical quantity is the projection of the spin angular momentum on the z axis, represented by operator $\boldsymbol{S_z}$. The eigenvalues are $+\hbar/2$ and $-\hbar/2$, corresponding to eigenstates $|\uparrow\rangle$ and $|\downarrow\rangle$.

$$\boldsymbol{S_z}|\uparrow\rangle = (+\hbar/2)|\uparrow\rangle \quad \text{and} \quad \boldsymbol{S_z}|\downarrow\rangle = (-\hbar/2)|\downarrow\rangle$$

Given $|\uparrow\rangle = |0\rangle = \begin{pmatrix}1\\0\end{pmatrix}$ and $|\downarrow\rangle = |1\rangle = \begin{pmatrix}0\\1\end{pmatrix}$, we get $\boldsymbol{S_z} = (\hbar/2)\begin{pmatrix}1 & 0\\0 & -1\end{pmatrix} = (\hbar/2)\boldsymbol{\sigma_z}$, where we define Pauli matrix $\boldsymbol{\sigma_z} = \begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}$. $\Rightarrow$ $\boldsymbol{\sigma_z}|\uparrow\rangle = |\uparrow\rangle$ and $\boldsymbol{\sigma_z}|\downarrow\rangle = -|\downarrow\rangle$, obvious in the matrix form.

Here, we state without explanation that the Pauli matrices for $\boldsymbol{S_x} = (\hbar/2)\boldsymbol{\sigma_x}$ and $\boldsymbol{S_y} = (\hbar/2)\boldsymbol{\sigma_y}$ are, respectively, $\boldsymbol{\sigma_x} = \begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}$ and $\boldsymbol{\sigma_y} = \begin{pmatrix}0 & -i\\i & 0\end{pmatrix}$.

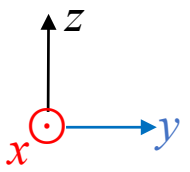


In-class exercise: Show that the eigenvalues of $\boldsymbol{S_x}$ (or $\boldsymbol{\sigma_x}$) are indeed $+\hbar/2$ and $-\hbar/2$ (or $+1$ and -1), and that the corresponding eigenstates in the basis of $|\uparrow\rangle$ and $|\downarrow\rangle$ are

$|\odot\rangle = |x_+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$ and $|\otimes\rangle = |x_-\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix} = \frac{1}{\sqrt{2}}(|\uparrow\rangle - |\downarrow\rangle)$.

Take-home exercise: Show that the eigenvalues of $\boldsymbol{S_y}$ (or $\boldsymbol{\sigma_y}$) are indeed $+\hbar/2$ and $-\hbar/2$ (or $+1$ and -1), and that the corresponding eigenstates in the basis of $|\uparrow\rangle$ and $|\downarrow\rangle$ are

$$|\rightarrow\rangle = |y_+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ i\end{pmatrix} = \frac{1}{\sqrt{2}}(|\uparrow\rangle + i|\downarrow\rangle) \text{ and } |\leftarrow\rangle = |y_-\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -i\end{pmatrix} = \frac{1}{\sqrt{2}}(|\uparrow\rangle - i|\downarrow\rangle).$$



Take-home exercise: Show that $\boldsymbol{\sigma_x}|\uparrow\rangle = |\downarrow\rangle$ and $\boldsymbol{\sigma_x}|\downarrow\rangle = |\uparrow\rangle$.

Side note: $\boldsymbol{\sigma_x}$ is the quantum NOT gate.

Important: An overall phase of a state vector has no physical consequences, e.g., $|\chi\rangle$ and $e^{i\varphi}|\chi\rangle$ represent the same state.

$|\leftarrow\rangle = |y_-\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -i\end{pmatrix}$ and $i|\leftarrow\rangle = i|y_-\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}i\\ 1\end{pmatrix}$ represent the same state, whose spin angular momentum projected onto y axis is $-\hbar/2$.

Take-home exercise: From

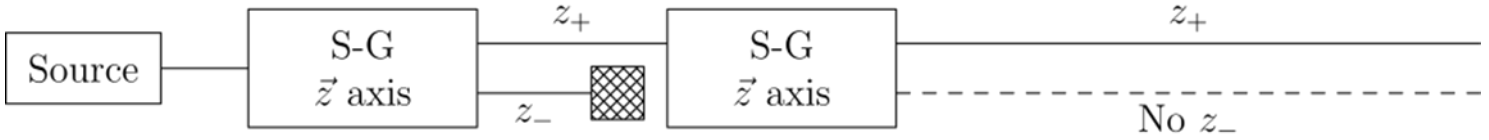
$|\rightarrow\rangle = |y_+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ i\end{pmatrix} = \frac{1}{\sqrt{2}}(|\uparrow\rangle + i|\downarrow\rangle)$ and $|\leftarrow\rangle = |y_-\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -i\end{pmatrix} = \frac{1}{\sqrt{2}}(|\uparrow\rangle - i|\downarrow\rangle)$, show

$$\boldsymbol{\sigma_x}|\rightarrow\rangle = i|\leftarrow\rangle \text{ and } \boldsymbol{\sigma_x}|\leftarrow\rangle = -i|\rightarrow\rangle.$$

Take-home exercise: Show $\boldsymbol{\sigma_z}|\odot\rangle = |\otimes\rangle$ and $\boldsymbol{\sigma_z}|\otimes\rangle = |\odot\rangle$; $\boldsymbol{\sigma_z}|\rightarrow\rangle = |\leftarrow\rangle$ and $\boldsymbol{\sigma_z}|\leftarrow\rangle = |\rightarrow\rangle$.

Side note: Pauli matrices $\boldsymbol{\sigma_x}$, $\boldsymbol{\sigma_y}$, and $\boldsymbol{\sigma_z}$ are known as the X (aka NOT), Y, and Z gates in quantum computing.

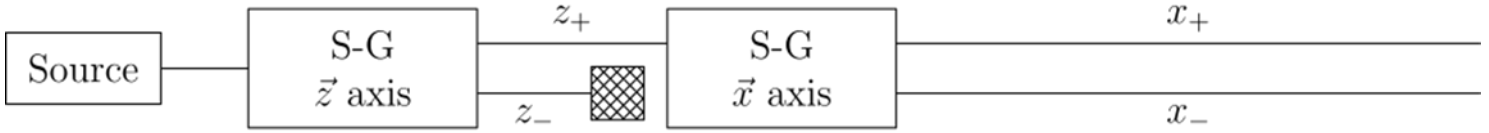
We now finally "know" enough to explain the sequential S-G experiments



https://en.wikipedia.org/wiki/Stern%E2%80%93Gerlach_experiment

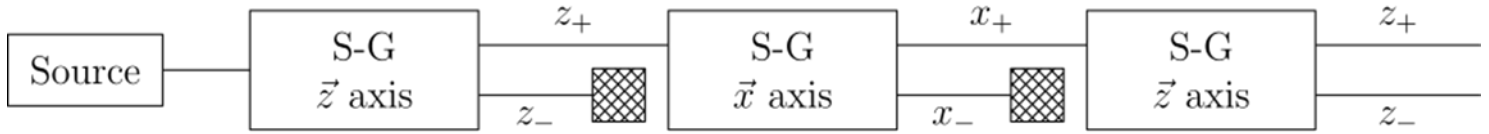
An electron is in a spin state $|\chi\rangle = c_\uparrow|\uparrow\rangle + c_\downarrow|\downarrow\rangle$, where $|c_\uparrow|^2 = |c_\downarrow|^2$ does not necessarily hold. Upon exiting the first S-G (z axis), the electron collapses to $|\uparrow\rangle$ or $|\downarrow\rangle$, with probabilities $|c_\uparrow|^2$ and $|c_\downarrow|^2$, respectively. Although $|c_\uparrow|^2 = |c_\downarrow|^2$ does not necessarily hold for individual electrons, equal counts of spin up and spin down measurements are expected if we do not skew the population.

Only the spin-up electrons are allowed to enter the second S-G (z axis), i.e., those are all in $|\uparrow\rangle$. Therefore, the only possible outcome is spin up.



From $|\odot\rangle = |x_+\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$ and $|\otimes\rangle = |x_-\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle - |\downarrow\rangle)$, we have $|\uparrow\rangle = \frac{1}{\sqrt{2}}(|x_+\rangle + |x_-\rangle)$ and $|\downarrow\rangle = \frac{1}{\sqrt{2}}(|x_+\rangle - |x_-\rangle)$. We thus have equal probability of detecting $|x_+\rangle$ and $|x_-\rangle$ for each electron.

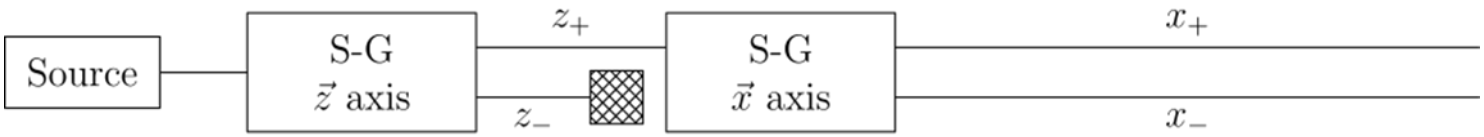
Exercise: write these expressions in the matrix form in the basis of $|\uparrow\rangle$ and $|\downarrow\rangle$.



This is now obvious from $|x_+\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$ and $|x_-\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle - |\downarrow\rangle)$.

We thus have equal probability of detecting $|z_+\rangle$ and $|z_-\rangle$ for each electron.

Common (or simultaneous) eigenstates



For an electron in $|\uparrow\rangle$, $\boldsymbol{\sigma_z}|\uparrow\rangle = |\uparrow\rangle$. From $\boldsymbol{\sigma_x}|\uparrow\rangle = |\downarrow\rangle = \frac{1}{\sqrt{2}}(|x_+\rangle - |x_-\rangle)$, which is neither $|x_+\rangle$ nor $|x_-\rangle$, we see that the eigenstate $|\uparrow\rangle$ of $\boldsymbol{\sigma_z}$ is not an eigenstate of $\boldsymbol{\sigma_x}$. Therefore, $\boldsymbol{S_z}$ and $\boldsymbol{S_x}$ cannot be determined at the same time. $\boldsymbol{S_z}$ and $\boldsymbol{S_x}$ do not have common (or simultaneous) eigenstates.

Since $\boldsymbol{\sigma_z}|\uparrow\rangle = |\uparrow\rangle$, we can write $\boldsymbol{\sigma_x}|\uparrow\rangle = |\downarrow\rangle = \boldsymbol{\sigma_x}\,(\boldsymbol{\sigma_z}|\uparrow\rangle) = (\boldsymbol{\sigma_x}\,\boldsymbol{\sigma_z})|\uparrow\rangle$, therefore $\boldsymbol{\sigma_x}\,\boldsymbol{\sigma_z}|\uparrow\rangle = |\downarrow\rangle$.
On the other hand, $\boldsymbol{\sigma_z}\,\boldsymbol{\sigma_x}|\uparrow\rangle = \boldsymbol{\sigma_z}\,(\boldsymbol{\sigma_x}\,|\uparrow\rangle) = \boldsymbol{\sigma_z}\,|\downarrow\rangle = -|\downarrow\rangle$.

Apparently, $\boldsymbol{\sigma_x}\,\boldsymbol{\sigma_z} \neq \boldsymbol{\sigma_z}\,\boldsymbol{\sigma_x}$. It appears that $\boldsymbol{\sigma_x}\,\boldsymbol{\sigma_z} = -\,\boldsymbol{\sigma_z}\,\boldsymbol{\sigma_x}$.

In-class exercise: Use matrix multiplication to show $\boldsymbol{\sigma_x}\,\boldsymbol{\sigma_z} = -\,\boldsymbol{\sigma_z}\,\boldsymbol{\sigma_x}$ is generally true.

Solution: Applying matrix multiplication to matrices $\boldsymbol{\sigma_x}$ and $\boldsymbol{\sigma_z}$, we get $\boldsymbol{\sigma_x}\,\boldsymbol{\sigma_z} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ and $\boldsymbol{\sigma_z}\,\boldsymbol{\sigma_x} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$. Therefore $\boldsymbol{\sigma_x}\,\boldsymbol{\sigma_z} = -\,\boldsymbol{\sigma_z}\,\boldsymbol{\sigma_x}$.

Homework 2:

Problem 1. (a) Find the eigenvalues and the corresponding eigenstates of $\boldsymbol{\sigma_x}\,\boldsymbol{\sigma_z}$. (b) Find the eigenvalues and the corresponding eigenstates of $\boldsymbol{\sigma_z}\,\boldsymbol{\sigma_x}$. (c) Compare your results with the eigenvalues and the corresponding eigenstates of $\boldsymbol{\sigma_y}$. Explain your observations.

Problem 2. Find a relation between $\boldsymbol{\sigma_y}$ and $\boldsymbol{\sigma_z}$, which is similar to $\boldsymbol{\sigma_x}\,\boldsymbol{\sigma_z} = -\,\boldsymbol{\sigma_z}\,\boldsymbol{\sigma_x}$.

The Pauli matrices do not commute with each other. Operators that do not commute do not have simultaneous eigenstates (obviously).

Take-home exercise: Use matrix multiplication to show $\boldsymbol{\sigma_x^2} = \boldsymbol{\sigma_y^2} = \boldsymbol{\sigma_z^2} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \mathbf{I}$. The unit matrix $\mathbf{I}$ can be written as simply 1.

$$\boldsymbol{\sigma_x^2} = \boldsymbol{\sigma_y^2} = \boldsymbol{\sigma_z^2} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \mathbf{I} \;\Rightarrow\; \boldsymbol{S_x^2} = \boldsymbol{S_y^2} = \boldsymbol{S_z^2} = \hbar^2/4$$

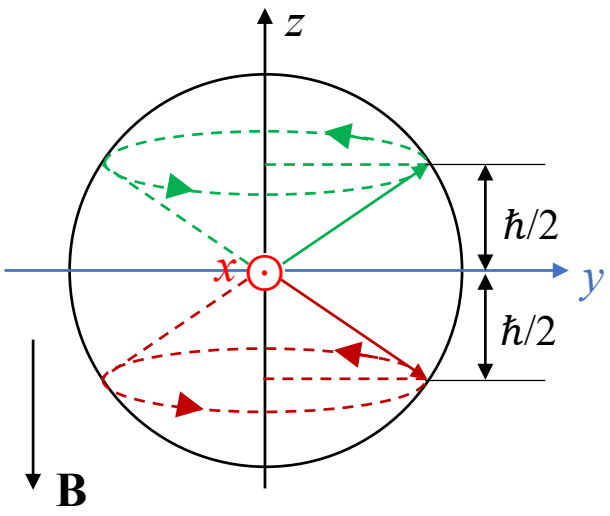
While $\boldsymbol{S_z}$, $\boldsymbol{S_x}$, and $\boldsymbol{S_y}$ cannot be determined at the same time, $\boldsymbol{S_x^2} = \boldsymbol{S_y^2} = \boldsymbol{S_z^2} = \hbar^2/4$ always holds, i.e., they are always determined and $\boldsymbol{S_x^2}$, $\boldsymbol{S_y^2}$, and $\boldsymbol{S_z^2}$ all have simultaneous eigenstates with each of $\boldsymbol{S_x}$, $\boldsymbol{S_y}$, and $\boldsymbol{S_z}$.

$$\boldsymbol{\sigma_x^2} = \boldsymbol{\sigma_y^2} = \boldsymbol{\sigma_z^2} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \mathbf{I} \Rightarrow \boldsymbol{S_x^2} = \boldsymbol{S_y^2} = \boldsymbol{S_z^2} = \hbar^2/4$$

For $\boldsymbol{S_z} = \pm\hbar/2$ (i.e. $\boldsymbol{\sigma_z} = \pm 1$), we have $\boldsymbol{S_x^2} = \boldsymbol{S_y^2} = \boldsymbol{S_z^2} = \hbar^2/4$ for both $\uparrow\rangle$ and $|\uparrow\rangle$. It is said that $\uparrow\rangle$ and $|\uparrow\rangle$ are degenerate in each of $\boldsymbol{S_x^2}$, $\boldsymbol{S_y^2}$, and $\boldsymbol{S_z^2}$. Similarly, $|\odot\rangle$ and $|\otimes\rangle$ are degenerate in each of these quantities. So are $|\rightarrow\rangle$ and $|\leftarrow\rangle$.

Relations between operators in quantum mechanics follow those between physical quantities known in classical physics.

Therefore, the total spin angular momentum $\boldsymbol{S}^2 = \boldsymbol{S_x^2} + \boldsymbol{S_y^2} + \boldsymbol{S_z^2} = 3\hbar^2/4$.
This can be loosely interpreted as the magnitude of the total spin angular momentum is always $S = |\mathbf{S}| = \frac{\sqrt{3}}{2}\hbar$. Finally, the picture of spin emerges:



In an applied DC magnetic field $\mathbf{B} = -B\hat{\mathbf{z}}$, $|\uparrow\rangle$ and $|\downarrow\rangle$ are the low- and high-energy states, respectively.
But, the field **B** itself does not align them; they can be considered as preceding around **B**.
In the presence of disturbance from the environment (sometimes called the bath), an electron does not stay in a definitive state for long.
At sufficiently low temperatures and after sufficiently long time, all electrons will be in the low-energy state $|\uparrow\rangle$.

More about Dirac notation

The ket $|\chi\rangle$ denotes a state independent of our choice of the basis.
$|\chi\rangle = c_{\odot}|\odot\rangle + c_{\otimes}|\otimes\rangle = c_{\rightarrow}|\rightarrow\rangle + c_{\leftarrow}|\leftarrow\rangle = c_{\uparrow}|\uparrow\rangle + c_{\downarrow}|\downarrow\rangle$

In the basis of $|\uparrow\rangle$ and $|\downarrow\rangle$ (or $|0\rangle$ and $|1\rangle$), $|\chi\rangle = \begin{pmatrix} c_{\uparrow} \\ c_{\downarrow} \end{pmatrix}$.

We now define the bra $\langle\chi| = (c_{\uparrow}^* \quad c_{\downarrow}^*)$. Obviously $\langle\chi|\chi\rangle = 1$. The state vector is normalized.

The basis of $|\uparrow\rangle$ and $|\downarrow\rangle$ (or $|0\rangle$ and $|1\rangle$) is said to be orthonormal because $\langle\uparrow|\uparrow\rangle = 1$, $\langle\downarrow|\downarrow\rangle = 1$, and $\langle\uparrow|\downarrow\rangle = 0$.

Similarly, the same is said of the basis set $|\odot\rangle$ and $|\otimes\rangle$ and the basis set $|\rightarrow\rangle$ and $|\leftarrow\rangle$.

Take-home exercise: Find $\langle\uparrow|\odot\rangle$ and $\langle\uparrow|\otimes\rangle$, and think about the sequential S-G measurements $\boldsymbol{\sigma_x}\,\boldsymbol{\sigma_z}$ again.

$\langle a|b\rangle = (a_0^* \quad a_1^*)\begin{pmatrix} b_0 \\ b_1 \end{pmatrix} = a_0^* b_0 + a_1^* b_1$ is the inner product of the two vectors $|a\rangle = \begin{pmatrix} a_0 \\ a_1 \end{pmatrix}$ and $|b\rangle = \begin{pmatrix} b_0 \\ b_1 \end{pmatrix}$.

Notice that the elements of the bra are complex conjugates of the corresponding ones in the ket.

Recall that the inner product $\langle a|b\rangle$ is the projection of $|b\rangle$ on to $|a\rangle$.
When project a vector onto a basis vector, you get the amplitude:
For arbitrary $|\chi\rangle = c_{\uparrow}|\uparrow\rangle + c_{\downarrow}|\downarrow\rangle$, we have $\langle\uparrow|\chi\rangle = c_{\uparrow}$ and $\langle\downarrow|\chi\rangle = c_{\downarrow}$.

Energy and time evolution of a quantum system

For a physical quantity Q represented by an operator $\mathbf{Q}$, with eigenvalues $q_0, q_1, q_2, \ldots, q_n, \ldots$, corresponding to eigenstates $|0\rangle, |1\rangle, \ldots, |n\rangle, \ldots$, we have $\mathbf{Q}|n\rangle = q_n|n\rangle$.

In the basis of $|0\rangle, |1\rangle, \ldots, |n\rangle, \ldots$, the matrix $\mathbf{Q}$ is diagonalized. This is obvious in the matrix form.

Energy E is such a special quantity that we give its operator a special name, the Hamiltonian $\boldsymbol{H}$, with eigenvalues $E_0, E_1, E_2, \ldots, E_n, \ldots$, corresponding to eigenstates $|0\rangle, |1\rangle, \ldots, |n\rangle, \ldots$
We have $\boldsymbol{H}|n\rangle = E_n|n\rangle$.

An energy eigenstate (i.e. a state with a definitive energy), $|n\rangle$, evolves in time following

$$|n(t)\rangle = e^{-i\frac{E_n}{\hbar}t}|n(0)\rangle = e^{-i\omega_n t}|n(0)\rangle, \text{ where } \omega_n = E_n/\hbar.$$

For a system in an energy eigenstate (i.e. a state with a definitive energy), $|n\rangle$, this phase evolution has no observable physical consequences.

For a system in a state that is a linear combination of energy eigenstates, $|\psi\rangle = \sum_n c_n|n\rangle$, each frequency evolves at a different frequency and beating happens.

This idea can be expressed in the matrix form, $|\psi(t)\rangle = \boldsymbol{U}(t)\,|\psi(0)\rangle$, where $\mathbf{U}(t)$ is a diagonalized matrix with the nth diagonal element being $e^{-i\omega_n t}$.

Too abstract? Let's make it clear with a simple 2-state system example:

Consider an electron in a DC magnetic field $\mathbf{B}$ in the $-z$ direction. Recall that the energy is $-\boldsymbol{\mu}\cdot\mathbf{B}$. Since the magnetic moment $\boldsymbol{\mu} \propto -\mathbf{S}$, the energy $\propto -S_z B$. Therefore, $\boldsymbol{S_z}$ and $\boldsymbol{H}$ have common eigenstates. For conformation to the quantum computing notations, and for extension to other 2-state systems, we now label the up- and down-spin states $|0\rangle$ and $|1\rangle$.
We then have $\boldsymbol{H}|0\rangle = \hbar\omega_0|0\rangle$ and $\boldsymbol{H}|1\rangle = \hbar\omega_1|1\rangle$

For an electron in a DC magnetic field, the up- and down-spin states, labeled $|0\rangle$ and $|1\rangle$, we have $\boldsymbol{H}|0\rangle = \hbar\omega_0|0\rangle$ and $\boldsymbol{H}|1\rangle = \hbar\omega_1|1\rangle$

$$|0(t)\rangle = e^{-i\omega_0 t}|0(0)\rangle \equiv e^{-i\omega_0 t}|0\rangle$$
$$|1(t)\rangle = e^{-i\omega_1 t}|1(0)\rangle \equiv e^{-i\omega_1 t}|1\rangle$$

The electron was initially in the state $|\odot\rangle = |x_+\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$ at $t = 0$. Since $\mathbf{B}$ // $-z$, it is not an eigenstate of $\boldsymbol{H}$. We now label it as $|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$. Let's follow the time evolution of this electron:

$$|\chi(t)\rangle = \frac{1}{\sqrt{2}}(e^{-i\omega_0 t}|0\rangle + e^{-i\omega_1 t}|1\rangle)$$

Let $\omega = \omega_1 - \omega_0$, and we have $|\chi(t)\rangle = \frac{1}{\sqrt{2}} e^{-i\frac{\omega_0+\omega_1}{2}t}(e^{i\frac{\omega}{2}t}|0\rangle + e^{-i\frac{\omega}{2}t}|1\rangle)$.

Inserting $|0\rangle = \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle)$ and $|1\rangle = \frac{1}{\sqrt{2}}(|+\rangle - |-\rangle)$ leads to

$$|\chi(t)\rangle = \frac{1}{2} e^{-i\frac{\omega_0+\omega_1}{2}t}[(e^{i\frac{\omega}{2}t} + e^{-i\frac{\omega}{2}t})|+\rangle + (e^{i\frac{\omega}{2}t} - e^{-i\frac{\omega}{2}t})|-\rangle]$$
$$= e^{-i\frac{\omega_0+\omega_1}{2}t}[(\cos\tfrac{\omega}{2}t)|+\rangle + (\sin\tfrac{\omega}{2}t)|-\rangle].$$

Overall phase with no observable physical consequences.

These are real amplitudes with observable physical consequences!

Questions:

If we measure electron spin in z-direction at time t, what are the probabilities of getting $+\hbar/2$ and $-\hbar/2$?

If we measure electron spin in x-direction at time t, what are the probabilities of getting $+\hbar/2$ and $-\hbar/2$?

In this case where $|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ at $t = 0$, it is said that the system is prepared in an initial state $|+\rangle$.

Since **B** // $-z$, it is not an eigenstate of $\boldsymbol{H}$, i.e., the system does not have a definitive energy.

The prepared initial state is a superposition of the high- and low-energy states (or spin-up and -down states).

In such cases, beating happens.

Questions:

If the system is prepared in an initial state $|0\rangle$, everything else the same as in the above case, how do the probabilities of measuring spin up and spin down change with time?

Will there be beating between $|0\rangle$ and $|1\rangle$?

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Questions:

If the system is prepared in an initial state $|0\rangle$, everything else the same as in the above case, how do the probabilities of measuring spin up and spin down change with time?
Will there be beating between $|0\rangle$ and $|1\rangle$?

Answers:

The probabilities of measuring spin up and spin down will remain 1 and 0, respectively.
There is no beating between $|0\rangle$ and $|1\rangle$.

The reason is that $|0\rangle$ is an eigenstate of $\boldsymbol{H}$, i.e., with a definitive energy, and therefore a definitive rate of phase evolution, ω_0.
Therefore, an energy eigenstate is said to be a stationary state.

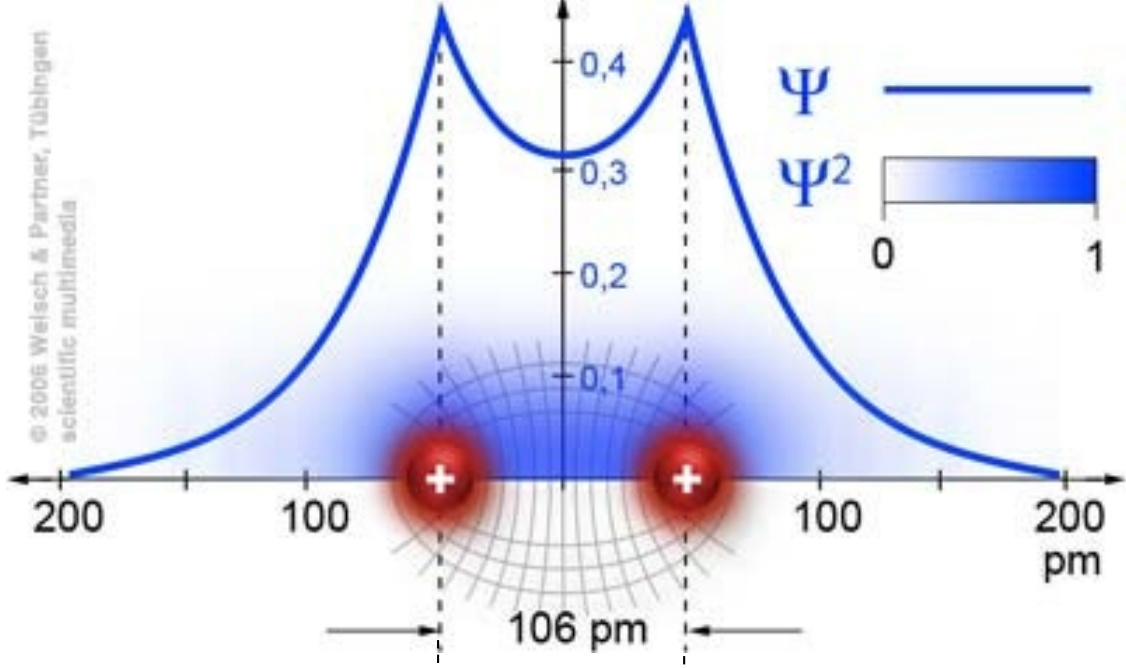
Will the electron remain in $|0\rangle$ forever?
Yes and No. If $\boldsymbol{H} \propto -BS_z$ indeed, without any other contributions, then yes.
But, quantum computing would be too easy if this were the case.
There will always be disturbance from the environment, which add to the Hamiltonian.

The chemical bond of H_2^+ is also a 2-state system

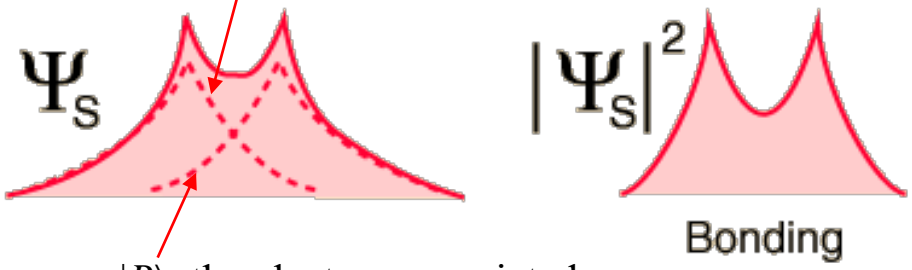
The electron is shared by the two protons, resulting in two stationary states:

Bonding: $|0\rangle = \frac{1}{\sqrt{2}}(|L\rangle + |R\rangle)$ and

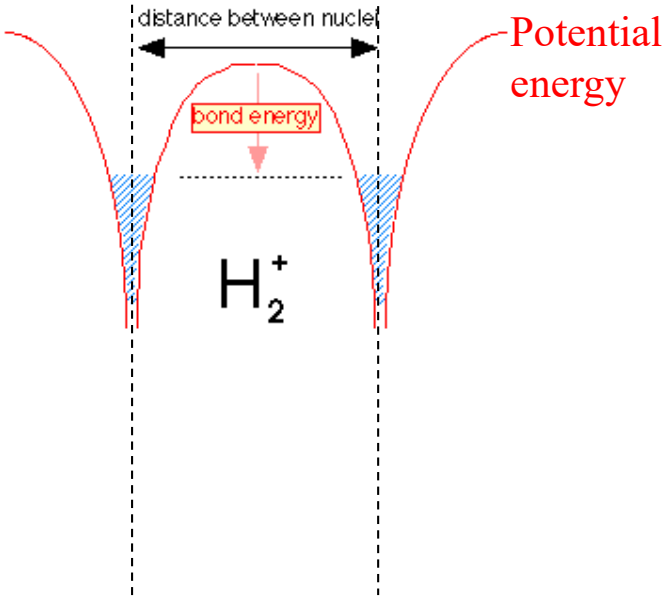
Antibonding: $|1\rangle = \frac{1}{\sqrt{2}}(|L\rangle - |R\rangle)$



$|L\rangle$: the electron associated with the left H atom



$|R\rangle$: the electron associated with the right H atom

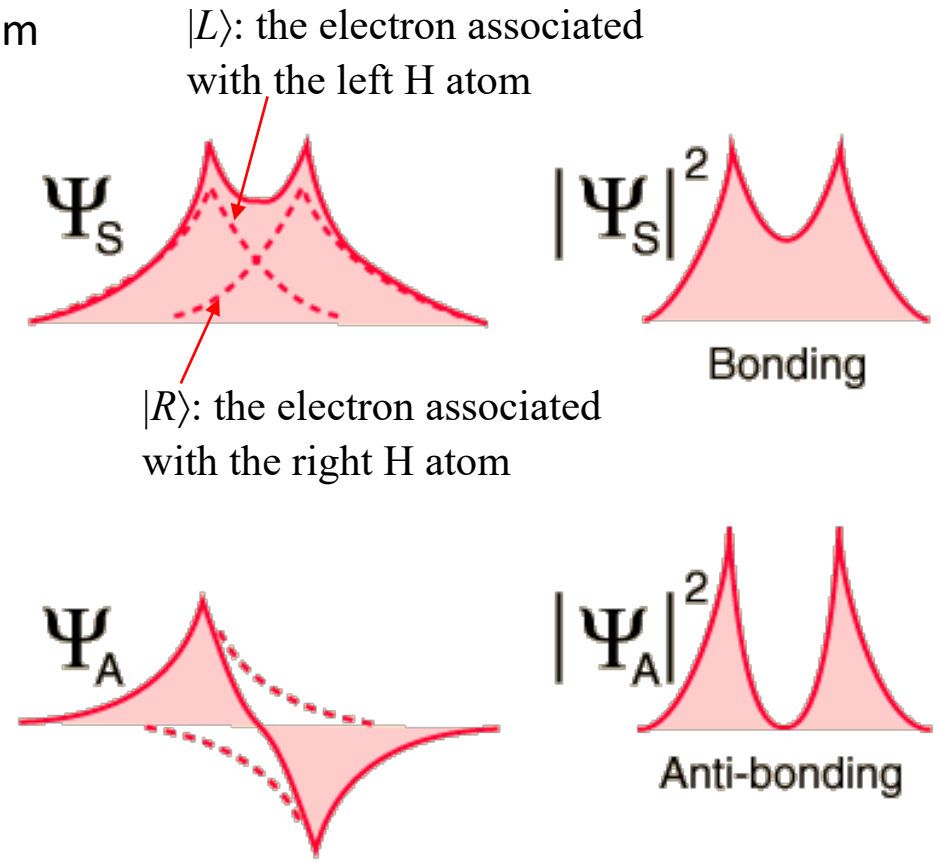


The chemical bond of H_2^+ is also a 2-state system

The electron is shared by the two protons, resulting in two stationary states:

Bonding: $|0\rangle = \frac{1}{\sqrt{2}}(|L\rangle + |R\rangle)$, lower-energy, symmetric

Antibonding: $|1\rangle = \frac{1}{\sqrt{2}}(|L\rangle - |R\rangle)$, higher-energy, antisymmetric



Questions:

If we prepare an H_2^+ in an initial state $|L\rangle$ at $t = 0$ and measure whether the electron is associated with the left or right proton, how do the probabilities of measuring left and right change with time? What if we prepare the H_2^+ in $|0\rangle$ at $t = 0$?

Answers:

If we prepare an H_2^+ in $|L\rangle$ at $t = 0$ and measure whether the electron is associated with the left or right proton, the probabilities of measuring left and right will oscillate back and forth at the frequency determined by half the energy difference between the bonding ($|0\rangle$) and antibonding ($|1\rangle$) states. What if we prepare the H_2^+ in $|0\rangle$ at $t = 0$, it will stay there forever. The probabilities are half/half for measuring left and right.

Quantities with continuous eigenvalues and Schrödinger equation

For a physical quantity Q represented by an operator $\mathbf{Q}$, with eigenvalues $q_0, q_1, \ldots, q_n, \ldots$, corresponding to eigenstates $|0\rangle, |1\rangle, \ldots, |n\rangle, \ldots$, we have $\mathbf{Q}|n\rangle = q_n|n\rangle$. This can be written in the matrix form.

If there are N eigenvalues corresponding to N eigenstates, the state space is N-dimensional.

The 2-state systems we discussed are the simplest. N may be infinity for the N-state system.

The spectrum of the eigenvalues may even be continuous!

Let's now consider the position of a particle in space.
For simplicity, let's say the space is 1-D and the positions is x, which is continuous. (Obviously, a particle in uniform, free space has equal probability to be at any x.)

Let $|x\rangle$ be the state in which the particle is localized at x.

Recall that for 2-state systems, an arbitrary state $|\chi\rangle = c_0|0\rangle + c_1|1\rangle$.

For an system, an arbitrary state $|\psi\rangle = \sum_n c_n|n\rangle$.

From discrete to continuous, summation becomes integral

Similarly, for continuous x, an arbitrary state $|\psi\rangle = \int_{-\infty}^{\infty} dx\, \psi(x)\, |x\rangle$.

Here, for continuous x, $\psi(x)$ is the amplitude of $|x\rangle$ in $|\psi\rangle$, i.e., projection of $|\psi\rangle$ onto $|x\rangle$, just as c_n is to $|\psi\rangle = \sum_n c_n|n\rangle$ in the discrete case.

2-state: $c_0 = \langle 0|\chi\rangle$ and $c_1 = \langle 1|\chi\rangle$
Discrete: $c_n = \langle n|\psi\rangle$

by analogy

$\psi(x) = \langle x|\psi\rangle$

For continuous x

Question: What is the physical meaning of $|\psi(x)|^2$?

Question: What is the physical meaning of $|\psi(x)|^2$?

Answer: Just as $|c_n|^2 = |\langle n|\chi\rangle|^2$ is the probability of finding the system in state $|n\rangle$,
$|\psi(x)|^2 = |\langle x|\psi\rangle|^2$ is the probability of finding the system in state $|x\rangle$,
i.e., at location x.

You may have learned that $\psi(x)$ is the wave function.
As for discrete states, the wave function is to be normalized: $\int_{-\infty}^{\infty} dx|\psi(x)|^2 = 1$.

Note: Not all wave functions can be normalized this way. We will re-examine normalization later.

Let's now consider a particle in free space.
Potential energy same everywhere, set it to 0. The total energy is the kinetic energy.

Recall the following:

> Relations between operators in quantum mechanics follow those between the corresponding physical quantities known in classical physics.

momentum

Hamiltonian (energy) $\boldsymbol{H} = \frac{\boldsymbol{p}^2}{2m}$ ← mass

Obviously, $\boldsymbol{H}$ and $\boldsymbol{p}$ have simultaneous eigenstates. In the 1D case, two momenta $\pm p$ correspond to the same energy E, i.e., the two corresponding eigenstates are degenerate in energy.

momentum

Hamiltonian (energy) $\boldsymbol{H} = \frac{\boldsymbol{p}^2}{2m}$

mass

Obviously, $\boldsymbol{H}$ and $\boldsymbol{p}$ have simultaneous eigenstates. In the 1D case, two momenta $\pm p$ correspond to the same energy E, i.e., the two corresponding eigenstates are degenerate in energy.

momentum eigenvalue

$\boldsymbol{p}\,|p\rangle = p\,|p\rangle$

momentum operator

momentum eigenstate corresponding to eigenvalue p

The wave function of $|p\rangle$ is $\psi_p(x) = \langle x|p\rangle$.

$$|p\rangle = \int_{-\infty}^{\infty} dx\, \psi_p(x)\, |x\rangle.$$

Let's examine the time evolution of $|p\rangle(t) = \int_{-\infty}^{\infty} dx\, \psi_p(x,t)\, |x\rangle$.

Since $|p\rangle$ is an eigenstate of $\boldsymbol{H}$, $|p\rangle(t) = e^{-i\frac{E}{\hbar}t}|p\rangle(0) = e^{-i\omega t}|p\rangle(0)$, where $\omega = \frac{E}{\hbar}$,

$$\psi_p(x,t) = e^{-i\omega t}\,\psi_p(x,0) = e^{-i\omega t}\,\psi_p(x).$$

Classically, the particle moves at a constant speed $v = {}^{p}/_{m}$, therefore $\psi_p(x - vt, 0) = \psi_p(x,t)$.

$$\Rightarrow \quad \psi_p(x - vt, 0) = \psi_p(x - vt) = e^{-i\omega t}\,\psi_p(x).$$

$$\psi_p(x - vt, 0) = \psi_p(x - vt) = e^{-i\omega t}\,\psi_p(x).$$

We can immediately see $\psi_p(x,t) = e^{-i\omega(t-\frac{x}{v})} = e^{i(\frac{\omega}{v}x-\omega t)}$.

$$\frac{\omega}{v} = \frac{E/\hbar}{p/m} = \frac{\frac{p^2}{2m\hbar}}{p/m} = p/\hbar\,.$$

$\Rightarrow$ define $k = p/\hbar$

$$\psi_p(x,t) = e^{i(kx-\omega t)} \qquad \psi_p(x,0) = \psi_p(x) = e^{ikx}$$

There seems to be an obvious problem: $|\psi_p(x)|^2 = 1$ and therefore $\int_{-\infty}^{\infty} dx\,|\psi_p(x)|^2 = \infty$.

We need to re-examine normalization.

For a physical quantity Q represented by an operator $\mathbf{Q}$, with N discrete eigenvalues $q_1, q_2, \ldots, q_n, \ldots$, corresponding to N eigenstates $|0\rangle, |1\rangle, \ldots, |n\rangle, \ldots$, we have $\mathbf{Q}|n\rangle = q_n|n\rangle$. This can be written in the matrix form.

The state space is N-dimensional, and N may be infinity.

The orthonormal condition is formally written as $\langle n|n'\rangle = \delta_{n,n'} \equiv \begin{cases} 0, & n \neq n' \\ 1, & n = n' \end{cases}$.

But, how do we handle situations where the eigenvalue spectrum is continuous?

For eigenstates with a discrete eigenvalue spectrum , the orthonormal condition is:

$$\langle n|n'\rangle = \delta_{n,n'} \equiv \begin{cases} 0, & n \neq n' \\ 1, & n = n' \end{cases}$$

How do we handle situations where the eigenvalue spectrum is **continuous**?

$$\langle x|x'\rangle = \delta(x-x') \equiv \begin{cases} 0, & x \neq x' \\ \infty, & x = x' \end{cases}$$

Notice that $\int_{-\infty}^{\infty} dx\ \delta(x-x') = 1$.

Example

The wave function of a particle exactly localized at a particular location x' is $\delta(x-x')$.

$$|\,x'\,\rangle = \int_{-\infty}^{\infty} dx\ \delta(x-x')|x\rangle$$

Since $\int_{-\infty}^{\infty} dx\ \delta(x-x')f(x) = f(x')$, we have $\int_{-\infty}^{\infty} dx\ \delta(x-x')|x\rangle = |x'\,\rangle$.

Consider another state $|x''\,\rangle$, in which the particle is localized at x''.

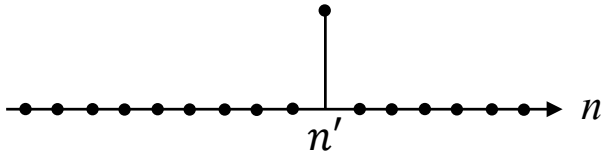
$$\langle x''|x'\rangle = \langle x''|\int_{-\infty}^{\infty} dx\ \delta(x-x')|x\rangle = \int_{-\infty}^{\infty} dx\ \delta(x-x')\,\langle x''|x\rangle$$

$$= \int_{-\infty}^{\infty} dx\ \delta(x-x')\,\delta(x-x'') = \delta(x'-x'') = \delta(x''-x')$$

$$x'' \to x \quad \Rightarrow \quad \langle x|x'\rangle = \delta(x-x')$$

This exercise is to show consistency of the definition of normalization for the continuous case, **not** attempting at any mathematical "proof".

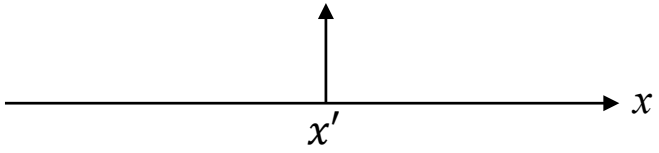
Discrete



$$\langle n|n'\rangle = \delta_{n,n'} \equiv \begin{cases} 0, & n \neq n' \\ 1, & n = n' \end{cases}$$

$$\sum_n \langle n|n'\rangle = \sum_n \delta_{n,n'} = 1$$

Continuous



$$\langle x|x'\rangle = \delta(x-x') \equiv \begin{cases} 0, & x \neq x' \\ \infty, & x = x' \end{cases}$$

$$\int_{-\infty}^{\infty} dx\, \langle x|x'\rangle = \int_{-\infty}^{\infty} dx\, \delta(x-x') = 1$$

Now you see, the two definitions of normalization are indeed equivalent.

Recall that $\delta(x-x')$ is the limiting case of a "pulse" (actually "packet" in space) at x'.

The definition is general, not just for position x. Applied to momentum: $\langle p|p'\rangle = \delta(p-p')$

Now we can re-examine the normalization of our momentum eigenstate $|p\rangle$:

$$|p\rangle = \int_{-\infty}^{\infty} dx\, \psi_p(x)\, |x\rangle.$$

For more details about dimensions/units, see the **FYI slides** below (not discussed in class).

Now we can re-examine the normalization of our momentum eigenstate $|p\rangle$:

$$|p\rangle = \int_{-\infty}^{\infty} dx\, \psi_p(x)\, |x\rangle.$$

Let $\langle x|p\rangle = \psi_p(x) = c_p e^{ikx}$, where c_p is the normalization constant.

Taking conjugates for the bra

$$\langle p|p'\rangle = \int_{-\infty}^{\infty} dx\, \psi_p^*(x)\langle x| \int_{-\infty}^{\infty} dx'\, \psi_{p'}(x')|x'\rangle$$

$$= \int_{-\infty}^{\infty} dx c_p^* e^{-ikx}\langle x| \int_{-\infty}^{\infty} dx' c_{p'} e^{ik'x'}|x'\rangle$$

$$= \int_{-\infty}^{\infty} dx c_p^* e^{-ikx} \int_{-\infty}^{\infty} dx' c_{p'} e^{ik'x'}\langle x|x'\rangle$$

$$= \int_{-\infty}^{\infty} dx c_p^* e^{-ikx} \int_{-\infty}^{\infty} dx' c_{p'} e^{ik'x'}\, \delta(x'-x)$$

$$= \int_{-\infty}^{\infty} dx c_p^* e^{-ikx}\, c_{p'} e^{ik'x}$$

$$= \int_{-\infty}^{\infty} dx c_p^* c_{p'} e^{i(k'-k)x}$$

$$= 2\pi c_p^* c_{p'}\, \delta(k-k')$$

$$= 2\pi\hbar c_p^* c_{p'}\, \delta(p-p')$$

$$= 2\pi\hbar |c_p|^2\, \delta(p-p')$$

$$= \delta(p-p')$$

Notes

Using $|p\rangle = \int_{-\infty}^{\infty} dx\, \psi_p(x)\, |x\rangle$

Inserting $\psi_p(x) = c_p e^{ikx}$

Using $\langle x|x'\rangle = \delta(x'-x)$

Using $\int_{-\infty}^{\infty} dx'\, \delta(x'-x)f(x') = f(x), f(x') = e^{ik'x'}$

Using $\int_{-\infty}^{\infty} dx e^{i(k'-k)x} = 2\pi\, \delta(k-k')$

Using $\delta(ax) = \delta(x)/|a|$ and $p = \hbar k$

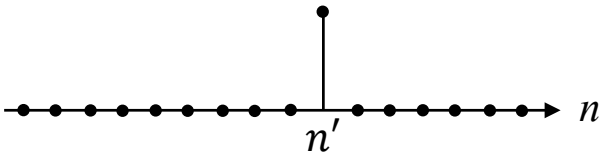
$c_{p'} = c_p$ when $p = p'$

Therefore, $2\pi\hbar|c_p|^2 = 1 \Rightarrow c_p = \frac{1}{\sqrt{2\pi\hbar}} \Rightarrow \boxed{\langle x|p\rangle = \psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ikx}}$

For more details about dimensions/units, see the **FYI slides** below (not discussed in class).

FYI: More on normalization of eigenstates of continuous spectra (not discussed in class)

Discrete: Quantity Q has eigenvalues q_n corresponding to eigenstates $|n\rangle$

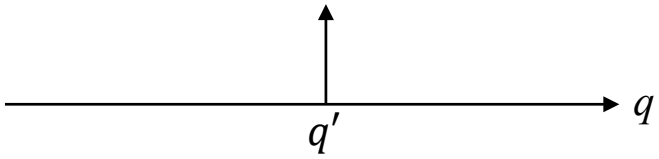


$$\langle n|n'\rangle = \delta_{n,n'} \equiv \begin{cases} 0, & n \neq n' \\ 1, & n = n' \end{cases}$$

$$\sum_n \langle n|n'\rangle = \sum_n \delta_{n,n'} = 1$$

$\langle n|n'\rangle = \delta_{n,n'}$ are dimensionless.

Continuous: Quantity Q has eigenvalues q corresponding to eigenstates $|q\rangle$



$$\langle q|q'\rangle = \delta(q-q') \equiv \begin{cases} 0, & q \neq q' \\ \infty, & q = q' \end{cases}$$

$$\int_{-\infty}^{\infty} dq\, \langle q|q'\rangle = \int_{-\infty}^{\infty} dq\, \delta(q-q') = 1$$

$\langle q|q'\rangle = \delta(q-q')$ are of dimension Q^{-1}.

So, it is reasonable to assign $|q\rangle$ the dimension $\mathrm{Q}^{-1/2}$

Now we see, $|x\rangle$ is of dimension $\mathrm{l}^{-1/2}$ (l is length),
and $|p\rangle$ is of dimension $\mathrm{p}^{-1/2}$ (p is momentum), if the spectrum for p is continuous.

Therefore, $\langle x|p\rangle$ is of dimension $(\mathrm{lp})^{-1/2}$.

$$\langle x|p\rangle = \psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ikx}$$

Recall that $\hbar$ has the dimension of angular momentum, which is $(\mathrm{lp})^{-1/2}$.
Thus we see, $\langle x|p\rangle$ is indeed of dimension $(\mathrm{lp})^{-1/2}$.

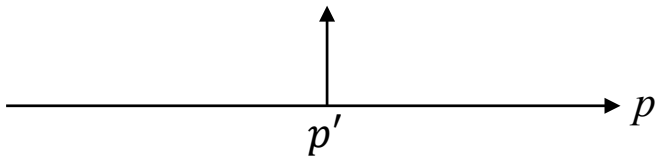
FYI (not discussed in class)

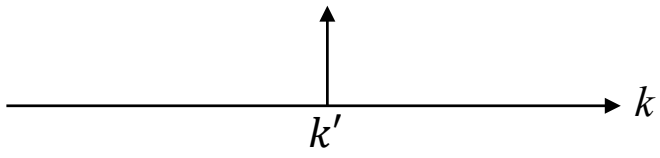
In general, for any Q with a continuous spectrum, $|q\rangle$ is of dimension $\mathrm{Q}^{-1/2}$ and $\langle x|q\rangle$ is of dimension $(\mathrm{lQ})^{-1/2}$.

On the other hand, for any Q with a discrete spectrum, $|n\rangle$ is of dimensionless and $\langle x|n\rangle$ is of dimension $\mathrm{l}^{-1/2}$.

With $p = \hbar k$, let's now examine $|p\rangle$ and $|k\rangle$.

$|p\rangle$ dimension $\mathrm{p}^{-1/2}$ (p is momentum),
$|k\rangle$ dimension $(\mathrm{l}^{-1})^{-1/2}$.





$$\langle p|p'\rangle = \delta(p-p') \equiv \begin{cases} 0, & p \neq p' \\ \infty, & p = p' \end{cases}$$

$$\langle k|k'\rangle = \delta(k-k') \equiv \begin{cases} 0, & k \neq k' \\ \infty, & k = k' \end{cases}$$

$$\int_{-\infty}^{\infty} dp\, \langle p|p'\rangle = \int_{-\infty}^{\infty} dp\, \delta(p-p') = 1$$

$$\int_{-\infty}^{\infty} dk\, \langle k|k'\rangle = \int_{-\infty}^{\infty} dk\, \delta(k-k') = 1$$

$\langle p|p'\rangle = \delta(p-p')$ are of dimension p^{-1}.

$\langle k|k'\rangle = \delta(k-k')$ are of dimension $(\mathrm{l}^{-1})^{-1}$.

$$\int_{-\infty}^{\infty} dp\, \langle p|p'\rangle = \int_{-\infty}^{\infty} dp\, \delta(p-p') = \int_{-\infty}^{\infty} d(\hbar k)\, \delta(\hbar k - \hbar k') = \int_{-\infty}^{\infty} dk\, \delta(k-k') = \int_{-\infty}^{\infty} dk\, \langle k|k'\rangle = 1$$

Using $\delta(ax) = \delta(x)/|a|$ and $p = \hbar k$

FYI (not discussed in class)

$$\int_{-\infty}^{\infty} dp\,\langle p|p'\rangle = \int_{-\infty}^{\infty} dp\,\delta(p-p') = \int_{-\infty}^{\infty} d(\hbar k)\,\delta(\hbar k-\hbar k') = \int_{-\infty}^{\infty} dk\,\delta(k-k') = \int_{-\infty}^{\infty} dk\,\langle k|k'\rangle = 1$$

Using $\delta(ax) = \delta(x)/|a|$ and $p = \hbar k$

$$\Rightarrow \qquad dp\,\langle p|p'\rangle = dk\,\langle k|k'\rangle$$

$$\Rightarrow \qquad \langle k|k'\rangle = \frac{dp}{dk}\langle p|p'\rangle = \hbar\langle p|p'\rangle \qquad \Rightarrow \qquad |k\rangle = \sqrt{\hbar}|p\rangle$$

$$\langle x|p\rangle = \psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}}\,e^{ikx} \qquad \Rightarrow \qquad \psi_k(x) \equiv \langle x|k\rangle = \sqrt{\hbar}\,\langle x|p\rangle = \frac{1}{\sqrt{2\pi}}\,e^{ikx}$$

Wave function of state $|p\rangle$

Wave function of state $|k\rangle$

An arbitrary state $|\psi\rangle = \int_{-\infty}^{\infty} dx\,\psi(x)\,|x\rangle$ can be expanded as a linear combination of states $|p\rangle$ or a linear combination of states $|k\rangle$.

Try to appreciate as much of the following as you can.
We will be kind of "derive" the **Fourier transform**.

$$\psi(x) = \langle x|\psi\rangle$$

insert

$$|\psi\rangle = \int_{-\infty}^{\infty} dx\,\psi(x)\,|x\rangle \qquad \Rightarrow \qquad |\psi\rangle = \int_{-\infty}^{\infty} dx\langle x|\psi\rangle\,|x\rangle = \int_{-\infty}^{\infty} dx|x\rangle\langle x|\psi\rangle$$

FYI (not discussed in class)

To expand an arbitrary state $|\psi\rangle = \int_{-\infty}^{\infty} dx \langle x|\psi\rangle\, |x\rangle = \int_{-\infty}^{\infty} dx |x\rangle\langle x|\psi\rangle$ as a linear combination of states $|p\rangle$, we need to find the "weights" $\langle p|\psi\rangle \equiv \phi_p(p)$.

$$\phi_p(p) \equiv \langle p|\psi\rangle = \langle p| \int_{-\infty}^{\infty} dx |x\rangle\langle x|\psi\rangle = \int_{-\infty}^{\infty} dx \langle p|x\rangle \langle x|\psi\rangle = \int_{-\infty}^{\infty} dx \, (\langle x|p\rangle)^* \langle x|\psi\rangle$$

insert

$$\langle x|p\rangle = \psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ikx}$$

insert

$$\psi(x) = \langle x|\psi\rangle$$

We put a subscript p here just to make $\phi_p(p)$ look different from $\phi(k)$, the weights of $|\psi\rangle$ when expanded onto $|k\rangle$.

$$\Rightarrow \quad \phi_p(p) \equiv \langle p|\psi\rangle = \int_{-\infty}^{\infty} dx \, [\psi_p(x)]^* \psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx e^{-ikx} \psi(x)$$

You see, this is simply the Fourier transform from "space domain" to "momentum domain":

$$\phi_p(p) \equiv \langle p|\psi\rangle = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx e^{-ikx} \psi(x)$$

Alternatively, we can expand $|\psi\rangle$ as a linear combination of states $|k\rangle$, with "weights" $\langle k|\psi\rangle \equiv \phi(p)$.

$$\phi(k) \equiv \langle k|\psi\rangle = \langle k| \int_{-\infty}^{\infty} dx |x\rangle\langle x|\psi\rangle = \int_{-\infty}^{\infty} dx \langle k|x\rangle \langle x|\psi\rangle = \int_{-\infty}^{\infty} dx \, (\langle x|k\rangle)^* \langle x|\psi\rangle$$

FYI (not discussed in class)

$$\phi(k) \equiv \langle k|\psi\rangle = \langle k| \int_{-\infty}^{\infty} dx |x\rangle\langle x| \psi\rangle = \int_{-\infty}^{\infty} dx \langle k|x\rangle \langle x|\psi\rangle = \int_{-\infty}^{\infty} dx \, (\langle x|k\rangle)^* \langle x|\psi\rangle$$

insert

insert

$$\psi_k(x) \equiv \langle x|k\rangle = \sqrt{\hbar}\,\langle x|p\rangle = \frac{1}{\sqrt{2\pi}} e^{ikx}$$

$$\psi(x) = \langle x|\psi\rangle$$

$$\Rightarrow \quad \phi(k) \equiv \langle k|\psi\rangle = \int_{-\infty}^{\infty} dx \, [\psi_k(x)]^* \psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-ikx} \psi(x)$$

This is simply the Fourier transform from "space domain" to "wavevector domain":

$$\phi(k) \equiv \langle k|\psi\rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-ikx} \psi(x)$$

Compare this with the Fourier transform to "momentum domain":

$$\phi_p(p) \equiv \langle p|\psi\rangle = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx e^{-ikx} \psi(x)$$

You see, there is a difference in the pre-factor.

These are the conclusions relevant to our following discussion on wave packets.

For simplicity, we considered a free particle in 1D. Its **normalized** wave function is a plane wave propagating in the x direction at a velocity $v = p/m = \hbar k/m$:

$$\psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ikx}$$

We now extend this into 3D. The **normalized** wave function is:

$$\psi_{\mathbf{p}}(\mathbf{r}) = \left(\frac{1}{\sqrt{2\pi\hbar}}\right)^3 e^{i\mathbf{k}\cdot\mathbf{r}}, \text{ where } \mathbf{r} = x\hat{\mathbf{x}} + y\hat{\mathbf{y}} + z\hat{\mathbf{z}} \text{ and } \mathbf{k} = k_x\hat{\mathbf{x}} + k_y\hat{\mathbf{y}} + k_z\hat{\mathbf{z}}$$

Just a plane wave propagating in the direction of $\mathbf{k}$ at a velocity $\mathbf{v} = \mathbf{p}/m = \hbar\mathbf{k}/m$.

Does this make sense?

A free particle in free space moving at a velocity $\mathbf{v} = \mathbf{p}/m = \hbar\mathbf{k}/m$, yet it all over the place with an equal probability $|\psi_p(\mathbf{r})|^2 = \left(\frac{1}{2\pi\hbar}\right)^3$ for all $\mathbf{r}$. The overall probability is $\int_{-\infty}^{\infty} dx |\psi_{\mathbf{p}}(x)|^2 = \infty$.

Yes, it makes sense.

We encountered similar situations in classical physics. Consider an electromagnetic (EM) plane wave propagating at a velocity $\mathbf{v} = (\frac{\omega}{k})\hat{\mathbf{k}}$. The intensity $|\mathbf{E}(\mathbf{r})|^2$ = constant for all $\mathbf{r}$. The overall power $\propto \int d^3\mathbf{r}\, |\mathbf{E}(\mathbf{r})|^2 = \infty$. We should have complained!

An EM pulse is a wave packet. Similarly, an electron is a wave packet.

To keep it simple, we again consider just one dimension (1D).

By Fourier transform, an arbitrary state $|\psi\rangle = \int_{-\infty}^{\infty} dx\, \psi(x)\, |x\rangle$ is expanded as a linear combination of plane wave states $|k\rangle$, with the "weights" $\langle k|\psi\rangle \equiv \phi(k)$:

$$\phi(k) \equiv \langle k|\psi\rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-ikx}\, \psi(x)$$

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk e^{ikx}\, \phi(k)$$

This is similar to the Fourier transform between a time domain signal and its frequency spectrum. Wavevector k is thus the spatial equivalent of angular frequency.

Recall that for a time-domain pulse, the product of pulse width and its spectrum width, $\Delta t\, \Delta\omega \sim 1$.

Similarly for a wave packet, the product of packet width and its spectrum width, $\Delta x\, \Delta k \sim 1$.

Since $p = \hbar k$, we have $\Delta x\, \Delta p \sim \hbar$.

The "uncertainty principle" of position and momentum

Wave packet dispersion

Now consider the propagation of a wave packet through space of time.

$$\psi(x,0) = \psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk e^{ikx}\, \phi(k)$$

$$\psi(x,t) = e^{-i\omega t}\, \psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk e^{i(kx-\omega t)}\, \phi(k)$$

If $\omega \propto |k|$, e.g., $\omega = c|k|$ for EM waves in free space,

$$E(x,t) = e^{-i\omega t} E(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk e^{ik(x-ct)}\, \phi(k).$$

The wave packet $E(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk e^{ikx}\, \phi(k)$ simply moves along x-direction at the phase velocity c without changing its shape. This is the dispersionless case.

For visualization, **closely** watch the first animation (A wave packet **without** dispersion) at https://en.wikipedia.org/wiki/Wave_packet.

For EM waves in a general medium or the electron (or any particle) wave $\psi(x,t)$, $\omega = \omega(k)$ is nonlinear. The wave packet will move along x-direction, but its shape will change and packet will broaden. This phenomenon is called dispersion.

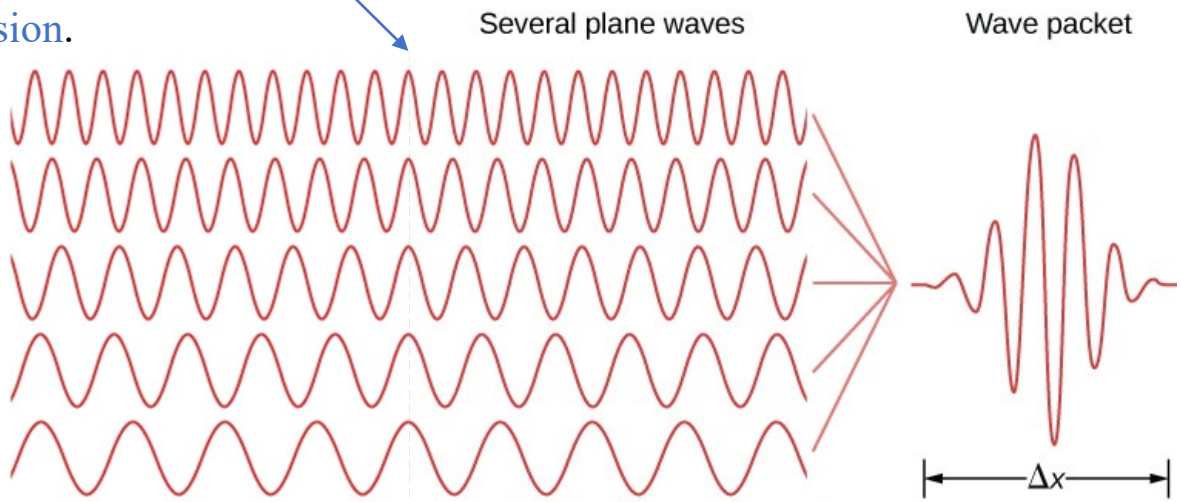
For visualization, **closely** watch the second animation (A wave packet **with** dispersion) at https://en.wikipedia.org/wiki/Wave_packet.

A true understanding of wave packets, interference, group velocity, uncertain principle, etc.

The center of the wave packet is where all plane waves of different k (or wavelength) are in phase.

(constructively interfere)

If $\omega \propto |k|$, all plane waves propagate at the phase velocity. Therefore, the center moves at the same speed. No dispersion.



plane waves of central wavevector k_c

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk e^{i[kx-\omega(k)t]}\, \phi(k)$$

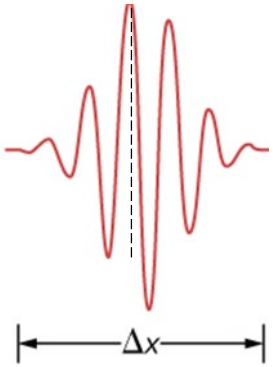


Illustration adapted from an image at

https://phys.libretexts.org/TextBooks_and_TextMaps/University_Physics/Book%3A_University_Physics_(OpenStax)/Map%3A_University_Physics_III_-_Optics_and_Modern_Physics_(OpenStax)/7%3A_Quantum_Mechanics/7.2%3A_The_Heisenberg_Uncertainty_Principle

The wave packet center x_c, constructive interference requires $\frac{\partial}{\partial k}[kx_c - \omega(k)t] = 0$.

$$\Rightarrow \quad x_c - \frac{d\omega}{dk} t = 0$$

$$\Rightarrow \quad x_c = \frac{d\omega}{dk} t$$

Thus, the center of the wave packet moves at a speed $\boxed{\frac{d\omega}{dk} \equiv v_g}$, called the group velocity.

With dispersion, while the center of the wave packet moves at the group velocity $\frac{d\omega}{dk} \equiv v_g$, the relative phase of a component plane wave k with regard to the plane wave of central wavevector k_c varies with time.

Therefore, the wave packet changes shape and usually broadens.

For visualization, again **closely** watch the second animation (A wave packet **with** dispersion) at https://en.wikipedia.org/wiki/Wave_packet.

For the electron (or any particle) wave $\psi(x,t)$, called the de Broglie wave, $\omega = \omega(k)$ is very nonlinear! $\omega \propto k^2 \Rightarrow$ very dispersive!

For visualization, **closely** watch animation at https://en.wikipedia.org/wiki/Wave_packet under *Gaussian wave packets in quantum mechanics*:

https://en.wikipedia.org/wiki/Wave_packet#/media/File:Wavepacket1.gif

This is the real (or imaginary) part **only**.

The wave function is complex. So for a full picture, watch the third animation under the same heading:

https://en.wikipedia.org/wiki/Wave_packet#/media/File:Wavepacket-a2k4-en.gif

Recall that $|\psi(x)|^2$ is the probability density. To see how the envelope of probability density propagates and evolves, watch the animation under the heading *Basic behaviors*: subheading *Dispersive*:

https://en.wikipedia.org/wiki/Wave_packet#/media/File:Guassian_Dispersion.gif

Schrödinger Equation

For a particle in free space, potential energy same everywhere, set to 0.

Recall the following:

> Relations between operators in quantum mechanics follow those between the corresponding physical quantities known in classical physics.

momentum

Hamiltonian (energy) $\boldsymbol{H} = \frac{\boldsymbol{p}^2}{2m}$ ← mass

Obviously, $\boldsymbol{H}$ and $\boldsymbol{p}$ have simultaneous eigenstates. In the 1D case, two momenta $\pm p$ correspond to the same energy E, i.e., the two corresponding eigenstates are degenerate in energy.

momentum eigenvalue

momentum operator → $\boldsymbol{p}\,|p\rangle = p\,|p\rangle$

momentum eigenstate corresponding to eigenvalue p

The wave function of $|p\rangle$ is $\psi_p(x) = \langle x|p\rangle$.

$$|p\rangle = \int_{-\infty}^{\infty} dx\, \psi_p(x)\, |x\rangle.$$

From the homogeneity of free space, i.e., equivalence of x and $x - vt$, we found $\psi_p(x,t)$, a plane wave. Now let's work out a differential equation for $\psi_p(x,t)$.

When talking about quantum beating, we mentioned:
An energy eigenstate (i.e. a state with a definitive energy), $|n\rangle$, in the case discrete spectra, evolves in time following

$$|n(t)\rangle = e^{-i\frac{E_n}{\hbar}t}|n(0)\rangle = e^{-i\omega_n t}|n(0)\rangle, \text{ where } \omega_n = E_n/\hbar.$$

The same is true for the continuous spectrum case:

Energy eigenvalue

$$|E\rangle(t) = e^{-i\frac{E}{\hbar}t}\,|E\rangle(0) = e^{-i\omega t}\,|E\rangle(0), \text{ where } \omega = E/\hbar.$$

Time varying factor

Stationary state, simply $|E\rangle$

This is actually the result of $i\hbar\frac{\partial}{\partial t}|E\rangle(t) = \boldsymbol{H}|E\rangle(t)$ when $\boldsymbol{H}$ does not depend on t, with $\boldsymbol{H}|E\rangle = E|E\rangle$.

Since $\boldsymbol{H}$ and $\boldsymbol{p}$ have simultaneous eigenstates,

$$|p\rangle(t) = e^{-i\frac{E}{\hbar}t}\,|p\rangle(t) = e^{-i\omega t}\,|p\rangle, \text{ where } \omega = E/\hbar \text{ and } E = p^2/2m = \hbar^2k^2/2m.$$

The remaining task is to deal with the stationary state: $\boldsymbol{p}\,|p\rangle = p\,|p\rangle$.

(From $|p\rangle$ that we already know for the free particle, figure out the operator $\boldsymbol{p}$.)

$$\boldsymbol{p}\,|p\rangle = p\,|p\rangle \quad \Rightarrow \quad \langle x|\,\boldsymbol{p}\,|p\rangle = p\,\langle x|p\rangle$$

Operator

Eigenvalue, just a number that can be taken out to the prefactor

Inserting $p\rangle = \int_{-\infty}^{\infty} dx\,\psi_p(x)\,|x\rangle$ and $\langle x|p\rangle = \psi_p(x)$, we get:

$$\langle x|\int_{-\infty}^{\infty} dx'\boldsymbol{p}\,\psi_p(x')\,|x'\rangle = p\,\psi_p(x).$$

Consider x' as the variable to be integrated over and x as a particular value

$$\Rightarrow \quad \int_{-\infty}^{\infty} dx'\boldsymbol{p}\,\psi_p(x')\,\langle x|x'\rangle = p\,\psi_p(x)$$

$$\Rightarrow \quad \int_{-\infty}^{\infty} dx'\boldsymbol{p}\,\psi_p(x')\,\delta(x'-x) = p\,\psi_p(x)$$

Using $\langle x|x'\rangle = \delta(x'-x)$

No state vectors in this equation now; we consider $\boldsymbol{p}\,\psi_p(x)$ as the operator operating on the function $\psi_p(x)$.

$$\Rightarrow \quad \boldsymbol{p}\,\psi_p(x) = p\,\psi_p(x)$$

How do we get this from the above equation?

This is the momentum eigenvalue equation in the wave function form.

We already know $\psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}}\,e^{ikx}$.

We also know very well that the derivative of an exponential function is proportional to itself.

Taking care of prefactors, we get:

$$\boxed{\boldsymbol{p} = -i\hbar\frac{\partial}{\partial x}}$$

$\boldsymbol{p} = -i\hbar\frac{\partial}{\partial x}$ $\Rightarrow$ Hamiltonian (energy) $\boxed{\boldsymbol{H} = \frac{\boldsymbol{p}^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}}$

Extend to 3D: $\boxed{\mathbf{p} = -i\hbar\nabla}$ $\boxed{\boldsymbol{H} = \frac{\mathbf{p}^2}{2m} = -\frac{\hbar^2}{2m}\nabla^2}$

Note on notation: When operating on wave functions, operators $\boldsymbol{Q}$ of are often denoted as $\hat{Q}$ to look different from the quantity Q. We started from treating operators as matrices, so we used bold $\boldsymbol{Q}$ to represent the operator for the quantity Q.

Now we have the **stationary** Schrödinger equation of a free particle in 1D:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x)$$ Exercise: Solve this equation.

Considering time variation:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t)$$ Exercise: Solve this equation.

Extend to 3D: $-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) = E\psi(\mathbf{r})$ $i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r},t)$

Exercise: Show that a de Broglie wave packet moves at the classical velocity $v = p/m$.

We have shown that eigenstate equations can be written in the wave function form for a free particle, i.e., the energy eigenstate equation:

$\mathbf{p} = -i\hbar\nabla \Rightarrow \boldsymbol{H} = \frac{\mathbf{p}^2}{2m} = -\frac{\hbar^2}{2m}\nabla^2$

$\boldsymbol{H}\,\psi(\mathbf{r}) = E\,\psi(\mathbf{r}) \Rightarrow -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) = E\,\psi(\mathbf{r})$ Stationary

$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t) = \boldsymbol{H}\,\psi(\mathbf{r},t) \Rightarrow i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r},t)$ Time-varying

These are the stationary & time-varying Schrödinger equations for a free particle.

Considering potential energy variation: $\boldsymbol{H} = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r},t) = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r},t)$, we have the general form

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r},t) + V(\mathbf{r},t)\,\psi(\mathbf{r},t)$$

Here, V is the potential **energy**.

Here, we only consider time-independent potential energy $V(\mathbf{r})$.
By separation of variables, we have

$\psi(\mathbf{r},t) = e^{-i\omega t}\,\psi(\mathbf{r})$

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + V(\mathbf{r},t)\,\psi(\mathbf{r},t) = E\,\psi(\mathbf{r})$$

$E = \hbar\omega$

We solve the stationary Schrödinger equation.

Important examples

Example 1: One-dimensional infinitely deep well

$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\,\psi(x)$ inside the well, $\psi(x) = 0$ outside.

Discussions: 1D standing wave, like that of a string or a transmission line with both ends shorted.

What about $n = 0$? What about $n = 0$?

Do ***H*** and and ***p*** have simultaneous eigenstates? What are the eigenstates of ***p***? "Good" quantum numbers.

$E_n \propto n^2$, $E_n \propto 1/a^2$.

Example 2: Three-dimensional hard-wall box

Discussions: degeneracy.

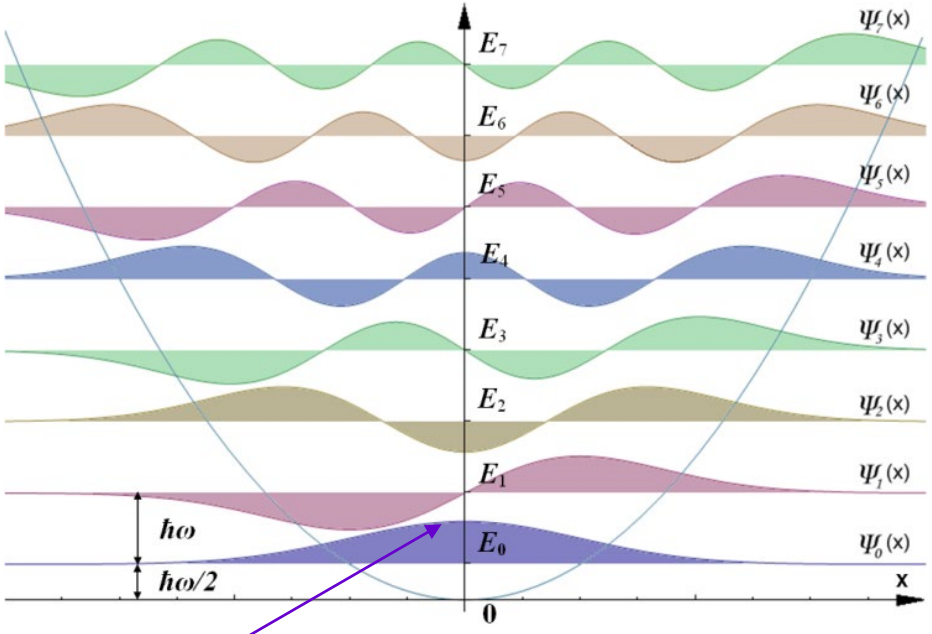
Homework 3

A particle is free in the x and y dimensions but is confined in $0 < z < c$. Find allowed stationary wave functions $\psi(x, y, z)$ and corresponding energies.
What if the particle is free in the x dimension but is confined in $0 < y < b$ and $0 < z < c$?
Hint: Think about metal waveguides for microwaves. You may label the wave functions (states) with "good" quantum numbers. Try to relate these states to the waveguide modes.

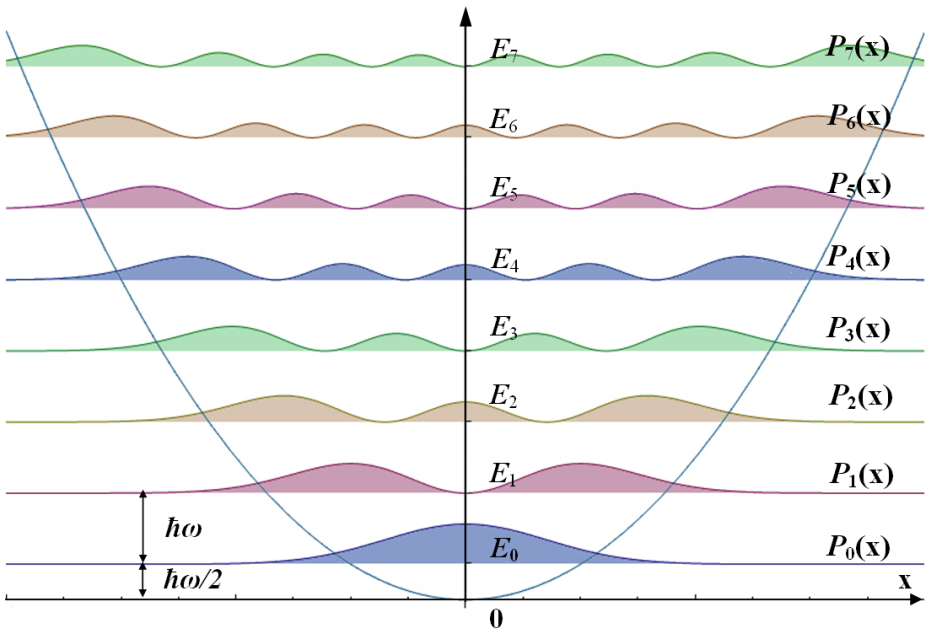
Example 3: One-dimensional harmonic oscillator

$$E_n = (n + \frac{1}{2})\hbar\omega_0$$

Wave functions



Probability distributions



$$\psi_0(x) = e^{-\frac{m\omega_0}{2\hbar}x^2}$$

Figures from Wikipedia page https://en.wikipedia.org/wiki/Quantum_harmonic_oscillator.

Discussions: What is $\psi_0(x,t)$? What is $\psi_n(x,t)$, given stationary $\psi_n(x)$?

Watch animation at Wikipedia page
https://en.wikipedia.org/wiki/Quantum_harmonic_oscillator

Example 4: One-dimensional finite-depth well

Discussions: Wave function tails and tunneling. Consider two wells close to each other.

Choice of setting the zero reference for energy: for your convenience.

As for the hard-wall cases, we can also have cases where the particle is free in on or two dimensions. EM wave analogy: dielectric cavities and waveguides. Notice the differences.

Example 5: H atom

$V(\mathbf{r}) = -\frac{e^2}{4\pi\varepsilon_0 r}$. $V(\infty) = 0$. Central force: angular momentum **L** conserved.

Recall that for spin, $\boldsymbol{H}$, $\boldsymbol{S}^2$, and $\boldsymbol{S}_z$ have simultaneous eigenstates, but $\boldsymbol{S}_x$, $\boldsymbol{S}_y$, and $\boldsymbol{S}_z$ do not. Similarly for orbital motion, $\boldsymbol{H}$, $\boldsymbol{L}^2$, and $\boldsymbol{L}_z$ have simultaneous eigenstates, but $\boldsymbol{L}_x$, $\boldsymbol{L}_y$, and $\boldsymbol{L}_z$ do not.

For spin, $S^2 = s(s+1)\hbar^2$, where s = ½ thus $S^2 = \frac{3}{4}\hbar^2$, and $S_z = m_s\hbar$, where $m_s = \pm\frac{1}{2}$: s and m_s are spin angular momentum quantum numbers.
For orbital motion, $L^2 = l(l+1)\hbar^2$, where $l = 0, 1, 2, \ldots$, and $L_z = m\hbar$, where $m = 0, \pm 1, \pm 2, \ldots, \pm l$, ($|m| < l$): l and m are orbital angular momentum quantum numbers.

Choose spherical coordinate system (r, θ, φ). Get radial and angular equations.

Choose spherical coordinate system (r, θ, φ). Get radial and angular equations by variable separation.

The solutions are $\psi_{nlm}(r,\theta,\varphi) = R_{nl}(r)Y_{lm}(\theta,\varphi)$, where the spherical harmonics Y_{lm} are solutions to angular momentum eigenvalue equations

$$\boldsymbol{L}^2 Y_{lm}(\theta,\varphi) = l(l+1)\hbar^2 Y_{lm}(\theta,\varphi),$$
$$\boldsymbol{L}_z Y_{lm}(\theta,\varphi) = m\hbar Y_{lm}(\theta,\varphi)$$

Further separate θ and φ: $Y_{lm}(\theta,\varphi) = \Theta_{lm}(\theta)\frac{1}{\sqrt{2\pi}}e^{im\varphi}$

Real valued

Normalization with regard to φ

$l = 0$, $m = 0$: s orbital. $\quad Y_{00}(\theta,\varphi) = \frac{1}{\sqrt{4\pi}}$

Angular momentum eigenvalues $L^2 = 0$, $L_z = 0$.

$l = 1$, $m = 0, \pm 1$: p orbitals

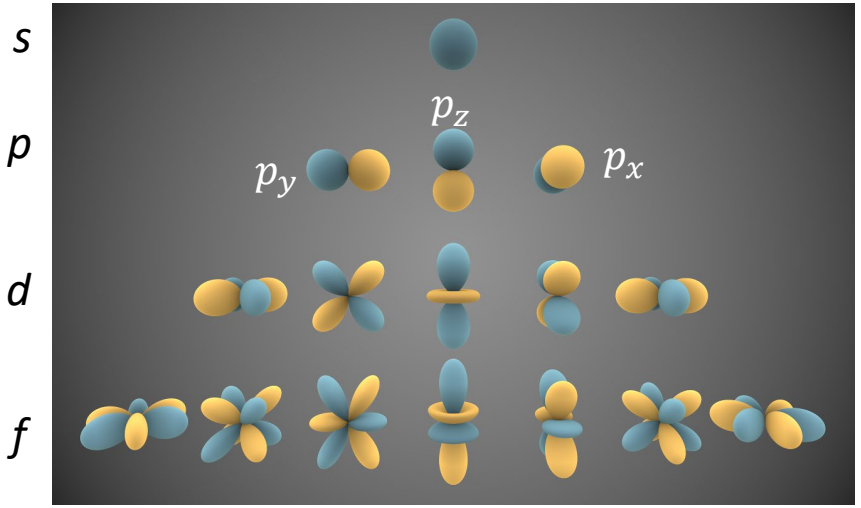
$l = 1$, $m = 0$: p_z orbital: angular momentum eigenvalues $L^2 = 2\hbar^2$, $L_z = 0$.

$$Y_{10}(\theta,\varphi) = \sqrt{\frac{3}{4\pi}}\cos\theta$$

$l = 1$, $m = \pm 1$: linear combinations form p_x and p_y orbitals: angular momentum eigenvalues $L^2 = 2\hbar^2$, $L_z = \pm\hbar$.

$l = 0, m = 0$: *s* orbital $\quad Y_{00}(\theta, \varphi) = \frac{1}{\sqrt{4\pi}}$

Angular momentum eigenvalues $L^2 = 0$, $L_z = 0$.



https://en.wikipedia.org/wiki/Spherical_harmonics

$l = 1, m = 0, \pm 1$: *p* orbitals

$l = 1, m = 0$: p_z orbital,

angular momentum eigenvalues $L^2 = 2\hbar^2$, $L_z = 0$.

$$Y_{10}(\theta, \varphi) = \sqrt{\frac{3}{4\pi}} \cos\theta = p_z$$

$l = 1, m = \pm 1$: linear combinations form **real-valued** p_x and p_y orbitals,

angular momentum eigenvalues $L^2 = 2\hbar^2$, $L_z = \pm\hbar$.

$$Y_{1,\pm 1}(\theta, \varphi) = \mp\sqrt{\frac{3}{8\pi}} \sin\theta \, e^{\pm i\varphi}$$

$$\Rightarrow \begin{cases} \frac{i}{\sqrt{2}}\left(Y_{1,-1} + Y_{1,-1}\right) = \sqrt{\frac{3}{4\pi}} \sin\theta \sin\varphi \\ \frac{1}{\sqrt{2}}\left(Y_{1,-1} - Y_{1,-1}\right) = \sqrt{\frac{3}{4\pi}} \sin\theta \cos\varphi \end{cases}$$

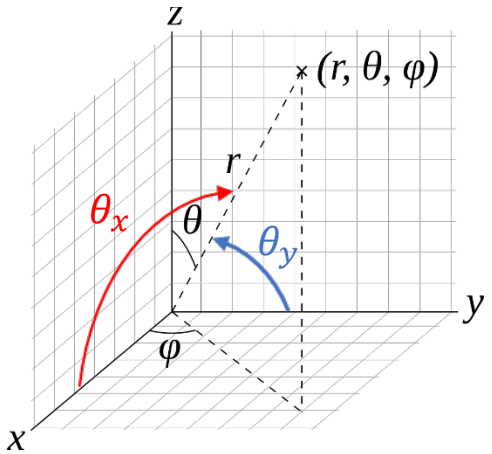
$|Y_{10}(\theta, \varphi)|^2$ $\qquad$ $|Y_{1,\pm 1}(\theta, \varphi)|^2$

http://mathworld.wolfram.com/SphericalHarmonic.html

You define polar angle from *y* axis, θ_y, and

polar angle from *x* axis, θ_x.

Easy to show $\begin{cases} \cos\theta_y = \sin\theta \sin\varphi \\ \cos\theta_x = \sin\theta \cos\varphi \end{cases}$

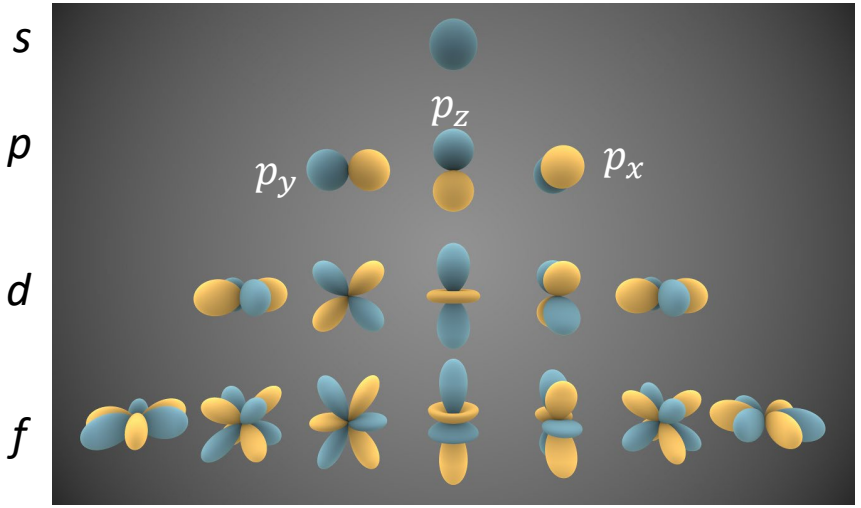


$l = 1, m = 0, \pm 1$: p orbitals

$l = 1, m = 0$: p_z orbital,
angular momentum eigenvalues $L^2 = 2\hbar^2$, $L_z = 0$.

$$Y_{10}(\theta, \varphi) = \sqrt{\frac{3}{4\pi}} \cos\theta \equiv p_z$$

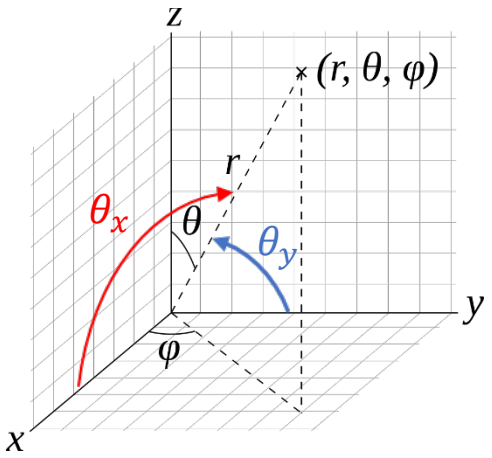
$l = 1, m = \pm 1$: linear combinations form **real-valued** p_x and p_y orbitals, angular momentum eigenvalues $L^2 = 2\hbar^2$, $L_z = \pm\hbar$.



https://en.wikipedia.org/wiki/Spherical_harmonics

Define polar angle from y axis, θ_y, and polar angle from x axis, θ_x.

$$\begin{cases} \frac{i}{\sqrt{2}}\left(Y_{1,-1} + Y_{1,1}\right) = \sqrt{\frac{3}{4\pi}} \sin\theta \sin\varphi = \sqrt{\frac{3}{4\pi}} \cos\theta_y \equiv p_y \\ \frac{1}{\sqrt{2}}\left(Y_{1,-1} - Y_{1,1}\right) = \sqrt{\frac{3}{4\pi}} \sin\theta \cos\varphi = \sqrt{\frac{3}{4\pi}} \cos\theta_x \equiv p_x \end{cases}$$



Interesting to note that
p_z is the eigenstate with $L^2 = 2\hbar^2$, $L_z = 0$
$(l = 1, m \equiv m_z = 0)$;
p_y is the eigenstate with $L^2 = 2\hbar^2$, $L_y = 0$
$(l = 1, m_y = 0)$;
p_x is the eigenstate with $L^2 = 2\hbar^2$, $L_x = 0$
$(l = 1, m_x = 0)$.

Define polar angle from y axis, θ_y, and polar angle from x axis, θ_x.

$$\cos\theta_y = \sin\theta \sin\varphi$$

$$\cos\theta_x = \sin\theta \cos\varphi$$

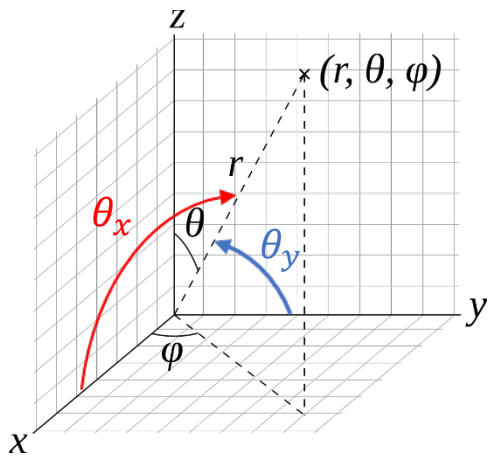
FYI: p_x, p_y, p_z orbitals and spherical harmonics

The p_x, p_y, p_z orbitals are real-valued. (Overall phase of one state irrelevant; the three are in phase.)

$$p_z = Y_{10}(\theta, \varphi) = \sqrt{\frac{3}{4\pi}} \cos\theta$$

$$\left.\begin{aligned} p_y &= \frac{i}{\sqrt{2}}\left(Y_{1,-1} + Y_{1,1}\right) = \sqrt{\frac{3}{4\pi}} \sin\theta \sin\varphi = \sqrt{\frac{3}{4\pi}} \cos\theta_y \\ p_x &= \frac{1}{\sqrt{2}}\left(Y_{1,-1} - Y_{1,1}\right) = \sqrt{\frac{3}{4\pi}} \sin\theta \cos\varphi = \sqrt{\frac{3}{4\pi}} \cos\theta_x \end{aligned}\right\}$$

$$\Rightarrow \begin{cases} Y_{1,1} = \dfrac{p_x + i p_y}{\sqrt{2}} \\ Y_{1,-1} = \dfrac{p_x - i p_y}{\sqrt{2}} \end{cases}$$



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$$\cos\theta_y = \sin\theta \sin\varphi$$

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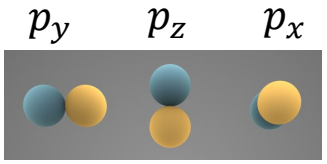


https://en.wikipedia.org/wiki/Spherical_harmonics

p_z is the eigenstate with $L^2 = 2\hbar^2$, $L_z = 0$ ($l = 1$, $m \equiv m_z = 0$);
p_y is the eigenstate with $L^2 = 2\hbar^2$, $L_y = 0$ ($l = 1$, $m_y = 0$);
p_x is the eigenstate with $L^2 = 2\hbar^2$, $L_x = 0$ ($l = 1$, $m_x = 0$).

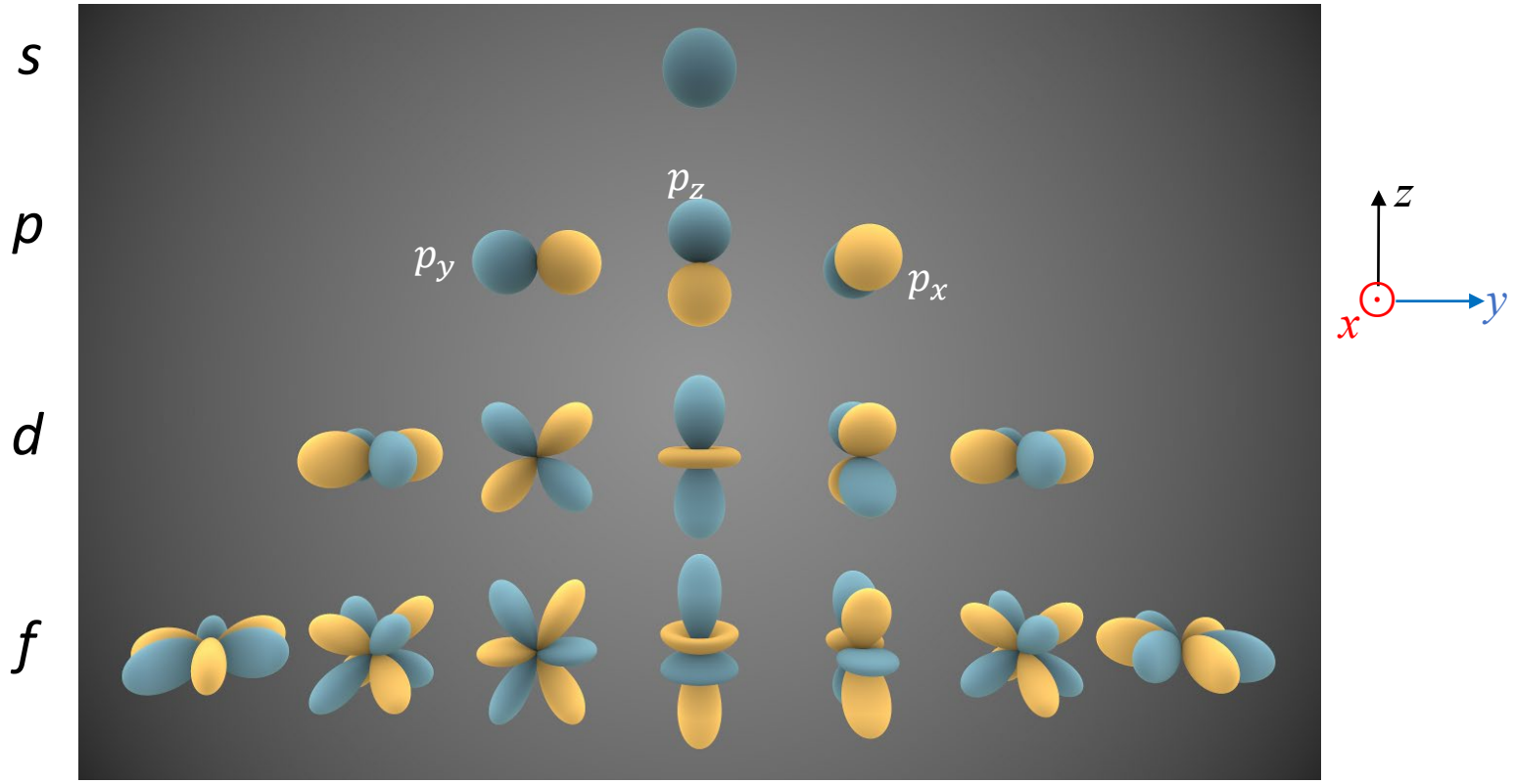
$l = 2, m = 0, \pm 1, \pm 2$: Five *d* orbitals

Angular momentum eigenvalues $L^2 = 6\hbar^2$.

For $m \neq 0$, linear combinations of $Y_{2,m}$ form **real-valued** *d* orbitals.

$l = 3, m = 0, \pm 1, \pm 2, \pm 3$: seven *f* orbitals

Angular momentum eigenvalues $L^2 = 12\hbar^2$.



https://en.wikipedia.org/wiki/Spherical_harmonics

These are solutions to the angular equation, which is the angular momentum eigenvalue equation.

The overall solutions are $\psi_{nlm}(r,\theta,\varphi) = R_{nl}(r)Y_{lm}(\theta,\varphi)$.

For all central forces, the angular solutions $Y_{lm}(\theta,\varphi)$ are the same.

For a general central force, the radial solutions $R_{nl}(r)$ correspond to energy eigenvalues E_{nl}.

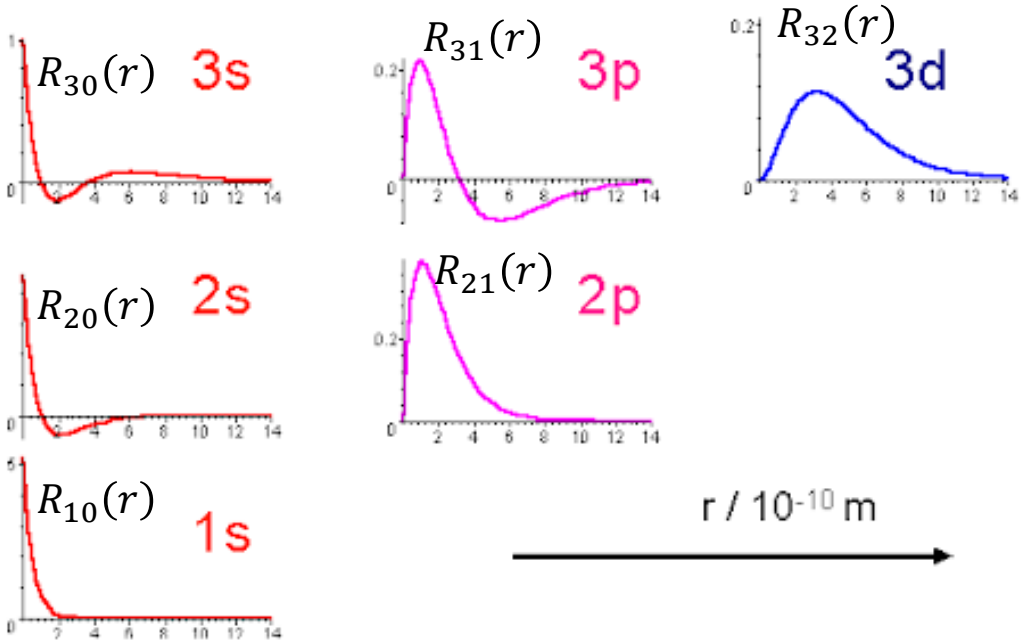
For the Coulomb force of a point charge, energy eigenvalues E_{nl} is degenerate for all l, thus simply E_n.

$n = 1, 2, 3, \ldots$

$l = 0, 1, 2, \ldots, n-1$

$$E_n = -\frac{1}{(4\pi\varepsilon_0)^2}\frac{me^4}{2\hbar^2}\frac{1}{n^2}$$

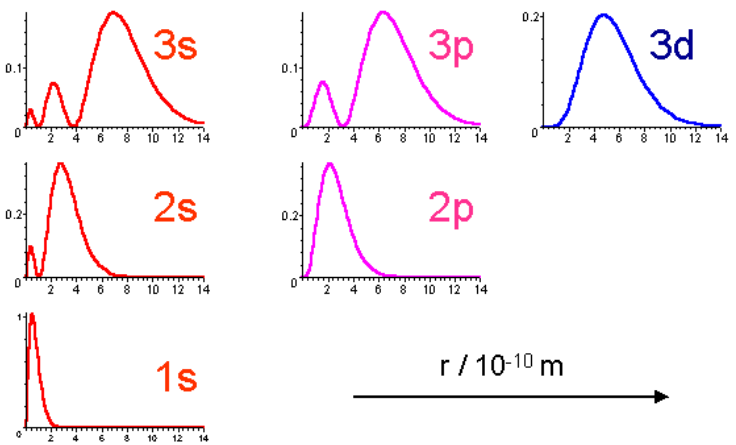
Electron wave functions of atomic hydrogen $R_{nl}(r)$



http://staff.mbi-berlin.de/hertel/physik3/chapter8/8.3html/01__99.png

$|rR_{nl}(r)|^2$

Electron density in atomic hydrogen w(r) = r² [R_{nl}(r)]²



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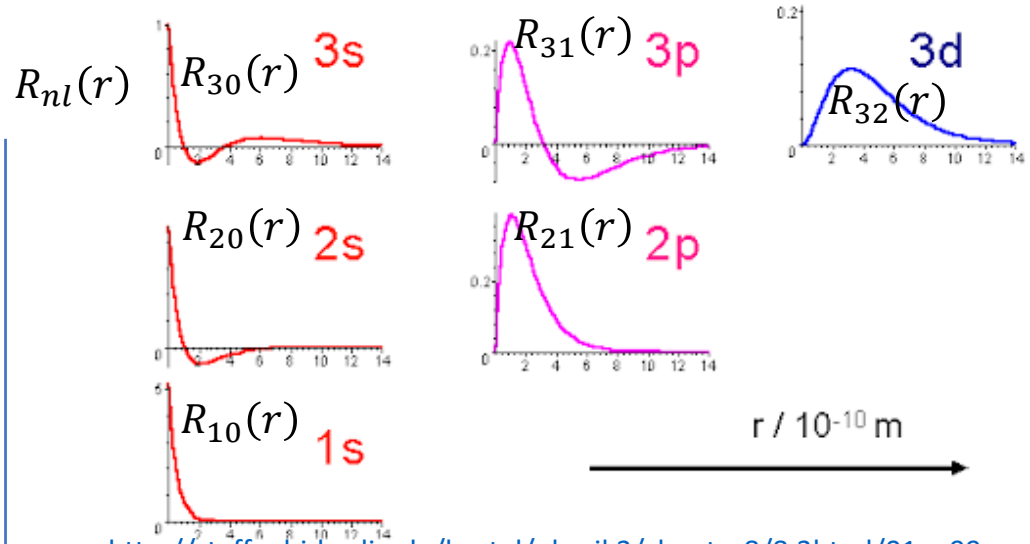
Visualization of $R_{nl}(r)$

$n = 1, 2, 3, \ldots$

$l = 0, 1, 2, \ldots, n-1$

Bohr radius $a_0 = 4\pi\varepsilon_0 \frac{\hbar^2}{me^2}$

$$E_n = -\frac{1}{(4\pi\varepsilon_0)^2}\frac{me^4}{2\hbar^2}\frac{1}{n^2} = -\frac{1}{4\pi\varepsilon_0}\frac{e^2}{2a_0}\frac{1}{n^2}$$



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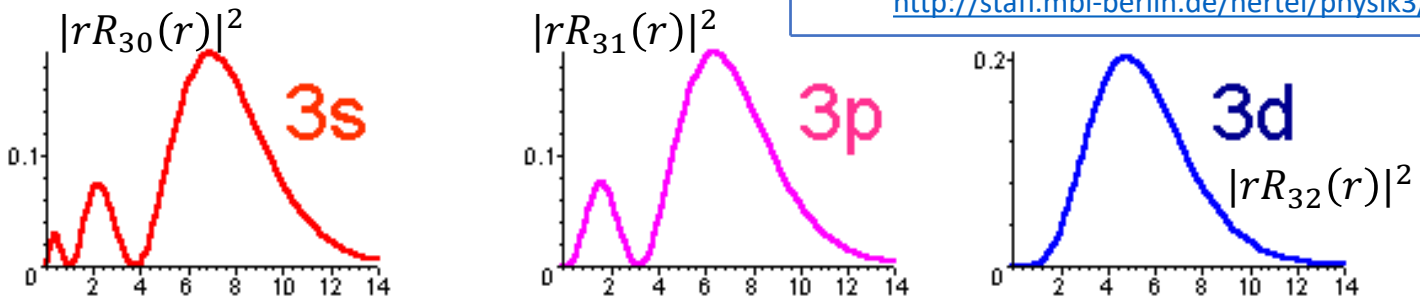
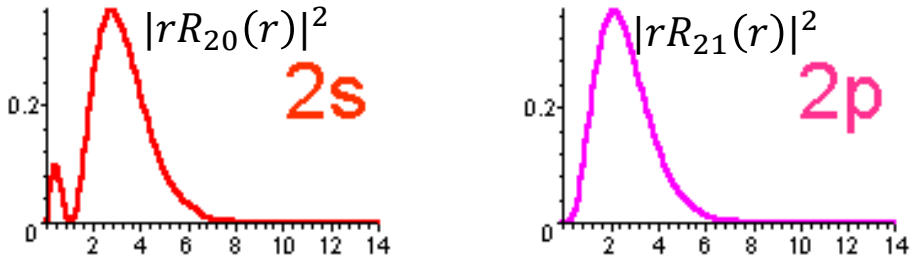
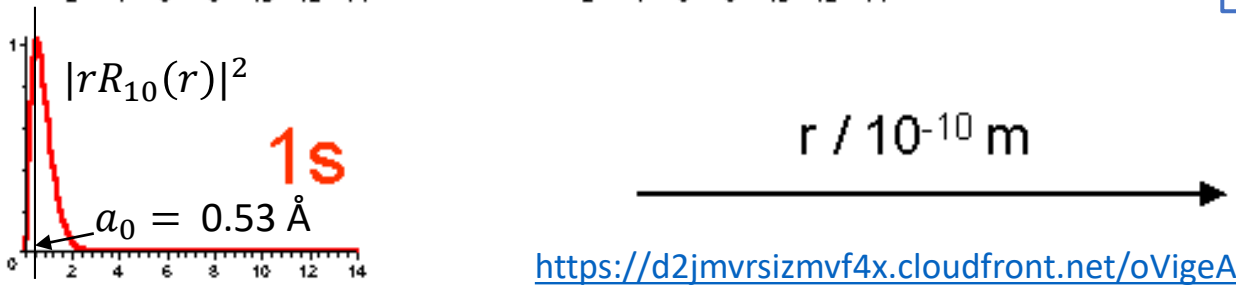
$|rR_{nl}(r)|^2$





$E_1 = -13.6$ eV

$a_0 = 0.53$ Å

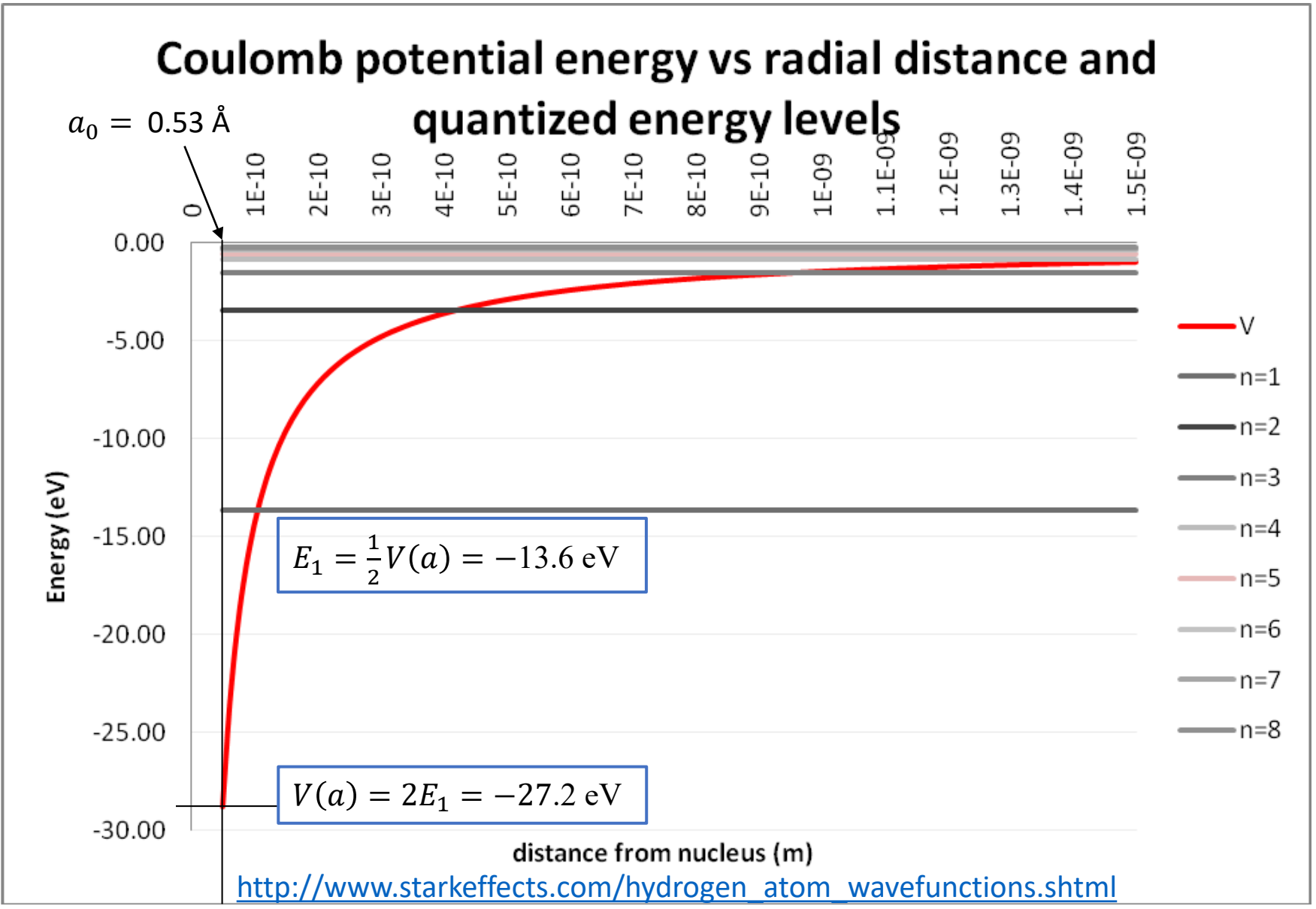


https://d2jmvrsizmvf4x.cloudfront.net/oVigeAgPQwC2STwkBOQr_01__100.png

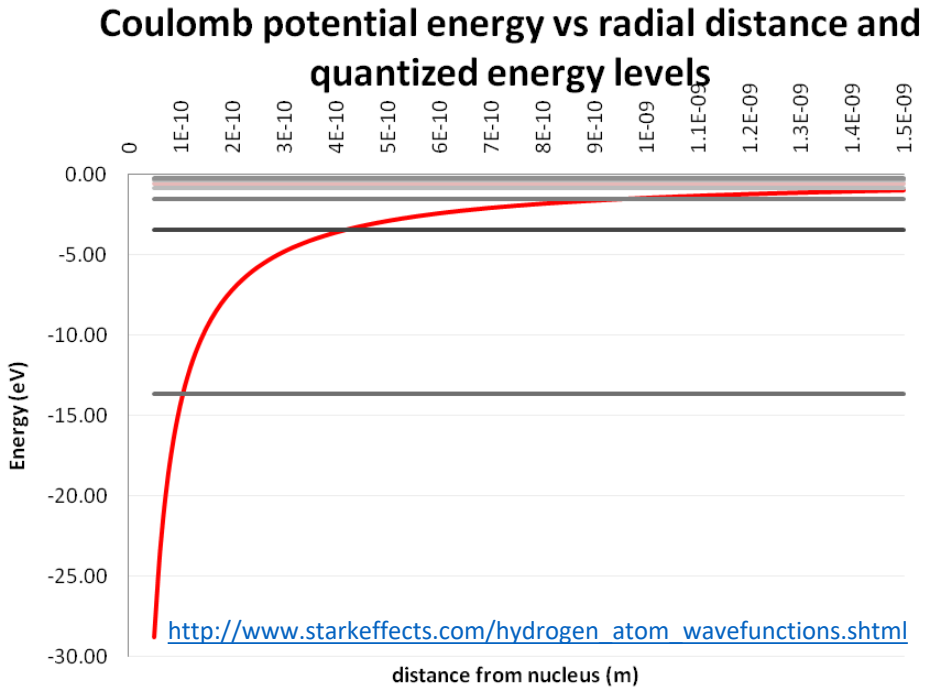
Visualization of the overall wave functions $\psi_{nlm}(r,\theta,\varphi) = R_{nl}(r)Y_{lm}(\theta,\varphi)$

	s ($\ell = 0$)	p ($\ell = 1$)			d ($\ell = 2$)					f ($\ell = 3$)						
	$m = 0$	$m = 0$	$m = \pm 1$		$m = 0$	$m = \pm 1$		$m = \pm 2$		$m = 0$	$m = \pm 1$		$m = \pm 2$		$m = \pm 3$	
	s	p_z	p_x	p_y	d_{z^2}	d_{xz}	d_{yz}	d_{xy}	$d_{x^2-y^2}$	f_{z^3}	f_{xz^2}	f_{yz^2}	f_{xyz}	$f_{z(x^2-y^2)}$	$f_{x(x^2-3y^2)}$	$f_{y(3x^2-y^2)}$
$n = 1$																
$n = 2$																
$n = 3$																
$n = 4$																
$n = 5$										…	…	…	…	…	…	…
$n = 6$					…	…	…	…	…	…	…	…	…	…	…	…

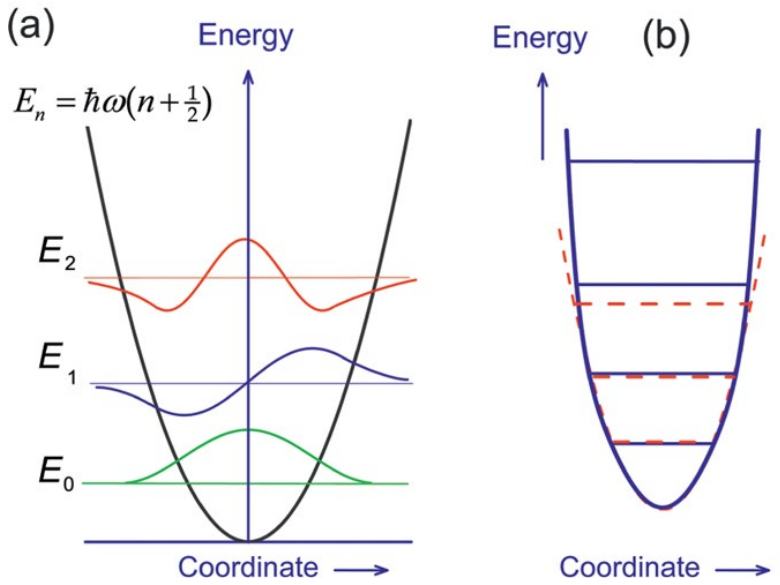
https://en.wikipedia.org/wiki/Atomic_orbital



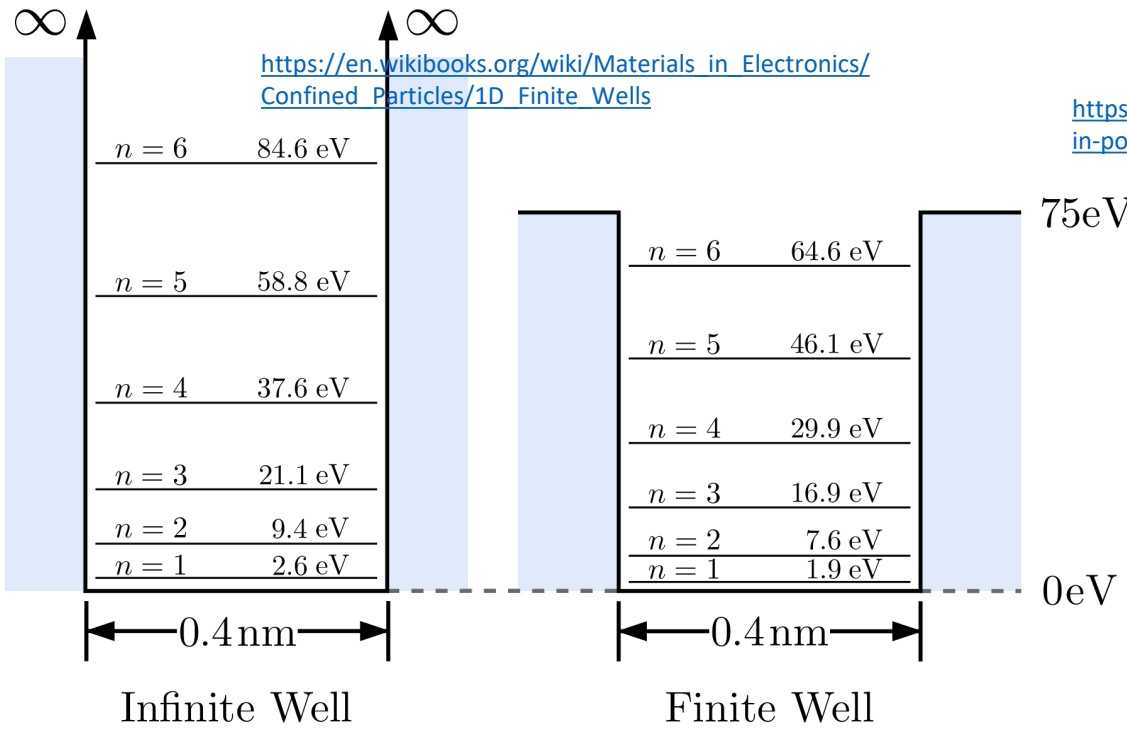
http://www.starkeffects.com/hydrogen_atom_wavefunctions.shtml

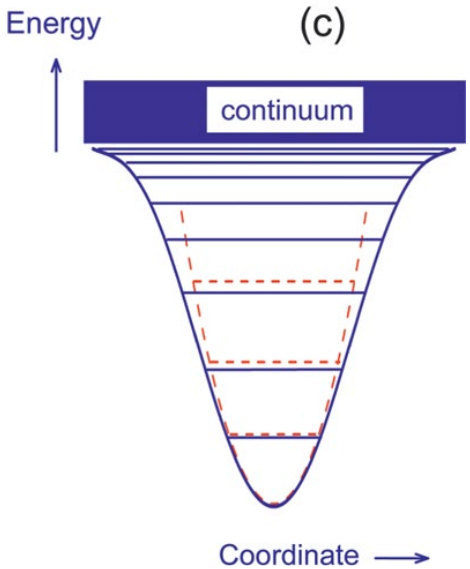


Potential well shapes and energy level distributions



https://www.cambridge.org/core/books/applied-nanophotonics/electrons-in-potential-wells-and-in-solids/D1A1D672320B55539DE286196D51EF47





Highlights and Remarks

Quantum mechanics is not weird.

We are familiar with waves, superposition, and coherence.

A possible reason it may look hard/weird:

For other waves, both the amplitude and the intensity are observable quantities.

In quantum mechanics, the amplitude *per se* is not observable while the analog of intensity is probability.

Analogy helps. Stationary states are like modes of electromagnetic wave.

But, we also notice differences.

Physical quantities are real. ⇒ Amplitudes of other waves are real. We use complex numbers as a math tool. For example, a single tone is the sum of a positive- and a negative-frequency Fourier component.

Amplitudes in quantum mechanics are complex.

Schrödinger equation vs. other wave equations.

$$\nabla^2\psi(\mathbf{r}) = -\frac{2m}{\hbar^2}[\hbar\omega - V(\mathbf{r})]\psi(\mathbf{r}) \quad \text{vs.} \quad \nabla^2\psi(\mathbf{r}) = -\frac{\omega^2}{c^2}n^2\psi(\mathbf{r}) \text{ for stationary states.}$$

A quantity e.g. E_z, V or I in 1D transmission line

Refractive index

There are no 1D dielectric cavities!

i vs. j as $\sqrt{-1}$.

$e^{-i\omega t}$ vs. $e^{j\omega t}$

$e^{i(kx-\omega t)}$ vs. $e^{j(\omega t-kx)}$

We are familiar with the vector space, linear algebra.

Again, complex amplitudes *per se* are not observable in quantum mechanics.

Amplitudes in quantum mechanics are complex.

Inner products involve taking complex conjugates.

(The bra is the conjugate transpose of the ket)

Complex amplitudes are used elsewhere for mathematical convenience.

Revisit H^+

Limited scope of this QM primer: one-particle

Revisit H_2^+

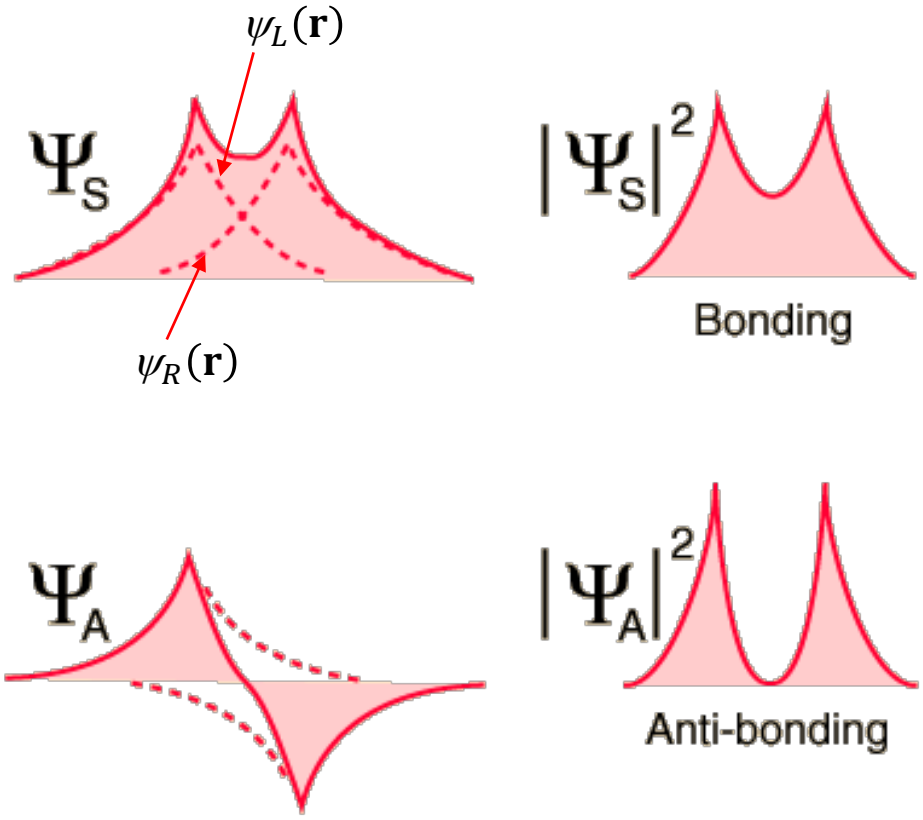
The electron is shared by the two protons, resulting in two stationary states:

Bonding: $|0\rangle = \frac{1}{\sqrt{2}}(|L\rangle + |R\rangle)$, lower-energy, symmetric

Antibonding: $|1\rangle = \frac{1}{\sqrt{2}}(|L\rangle - |R\rangle)$, higher-energy, antisymmetric

$|L\rangle$: the electron associated with the left H atom $\quad \langle \mathbf{r}|L\rangle = \psi_L(x)$

$|R\rangle$: the electron associated with the right H atom $\quad \langle \mathbf{r}|R\rangle = \psi_R(x)$



Convenient to take the two atomic orbitals (1s) centered at the two nuclei as the two basis vectors $|L\rangle$ and $|R\rangle$.

Question:

Do you see a problem with this choice of the basis set?

Revisit H_2^+

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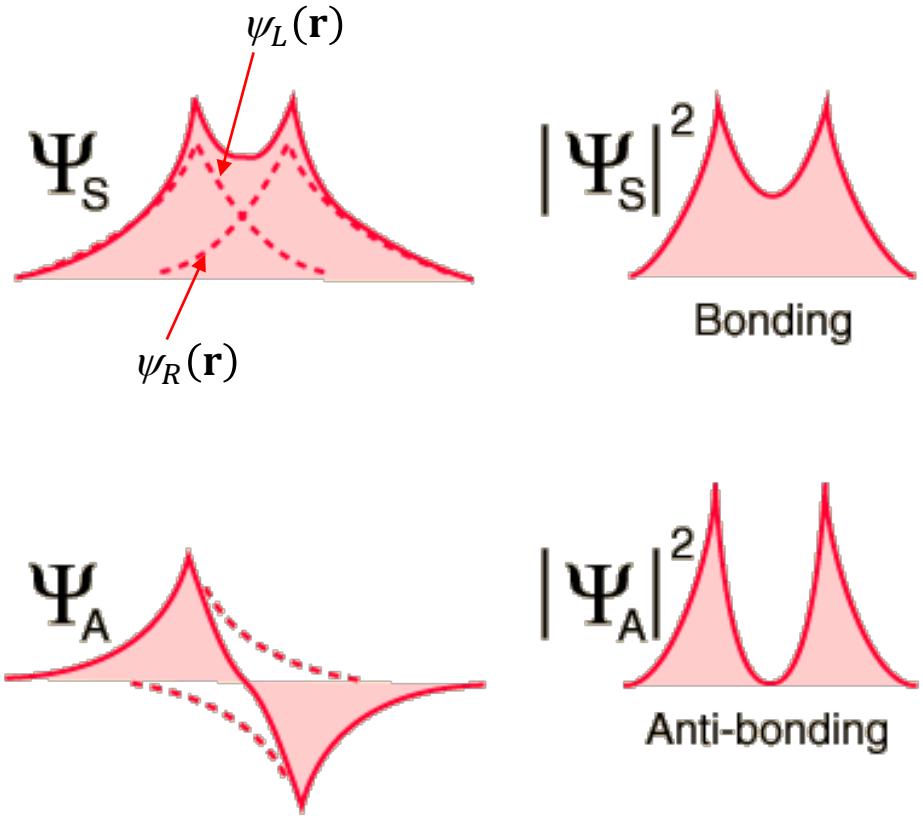

Convenient to take the two atomic orbitals (1s) centered at the two nuclei as the two basis vectors $|L\rangle$ and $|R\rangle$.

But, there is a problem: $\quad \langle L|R\rangle = \int d^3\mathbf{r}\,\psi_L^*(x)\,\psi_R(x) \neq 0$

Limited scope of this QM primer: one-particle

For example, another issue (approximation) w/ the above H_2^+ picture:

We kept the two protons fixed.

Homework 1

An abrupt pn junction is made by joining a uniformly n-doped region to a uniformly doped p-doped region. The dopant density of two regions are $N_D = 5 \times 10^{16}$ cm^{-3} and $N_D = 2 \times 10^{16}$ cm^{-3}, respectively.

Set the interface between the p and n regions at $x = 0$. Find the electron density $n(x)$, hole density $p(x)$, and electrostatic potential $\phi(x)$ as functions of x. Plot these functions to visualize them. The units for the horizontal and vertical axes of these plots must be specified.

Find the depletion widths x_n and x_p on the n and p side, respectively. Find the built-in voltage ϕ_i.

Note: The solutions will be the starting point of the mini project.

Due date Thu 1/30 okay?