# 14. Schrodinger's equation and unitary operations

$$|\psi(0)\rangle \rightarrow \boxed{U} \rightarrow |\psi(t)\rangle$$

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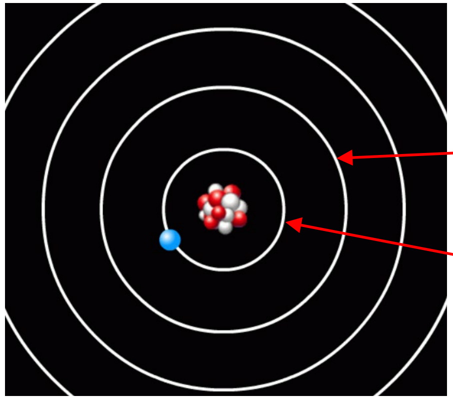
# Time evolution of the wavefunction

Up to this point we have considered the wavefunction to be static:



$|1\rangle$

$|0\rangle$

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

The wavefunction was just "given" to us from somewhere, and the only change that we could induce on the state was via a measurement

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \Rightarrow \boxed{\text{Measurement apparatus}}$$

$$p_0 = |\alpha|^2 \quad |\psi_0^{meas}\rangle = |0\rangle$$

$$|\psi_1^{meas}\rangle = |1\rangle \quad p_1 = |\beta|^2$$

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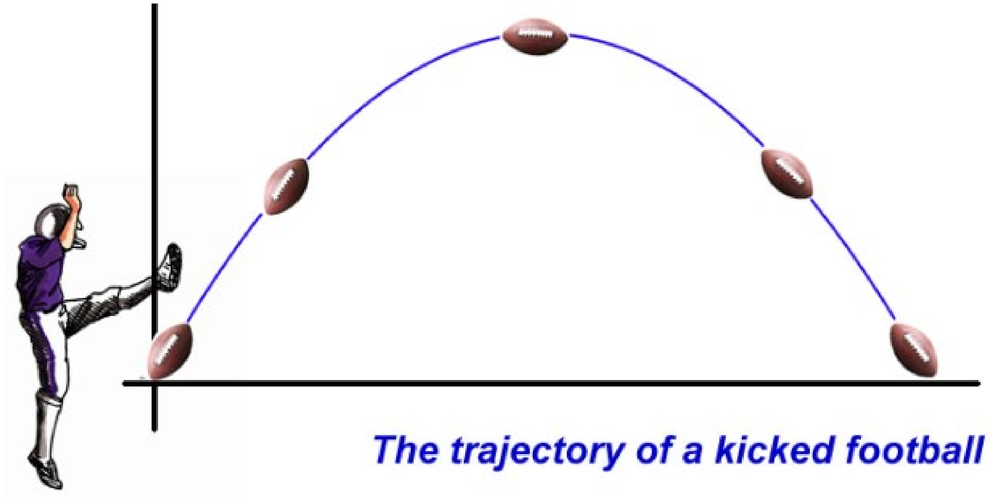
But just like classical physics, where the state (e.g. position, velocity etc.) can change in time $x(t), v(t)$ a quantum state can change in time.

A time-dependent quantum state is written by time-dependent coefficients.

$$|\psi(t)\rangle = \sum_{n=0}^{N} a_n(t) |n\rangle$$




The coefficients still always need to be normalized:

$$\langle \psi(t) | \psi(t) \rangle = 1 \qquad \sum_{n=0}^{N} |a_n(t)|^2 = 1$$

In the classical case, we can distinguish between cases where the state changes due to a "natural" evolution and "human intervention"

Quantum mechanics is exactly the same, the state evolution can happen "naturally" or due to "manipulation".

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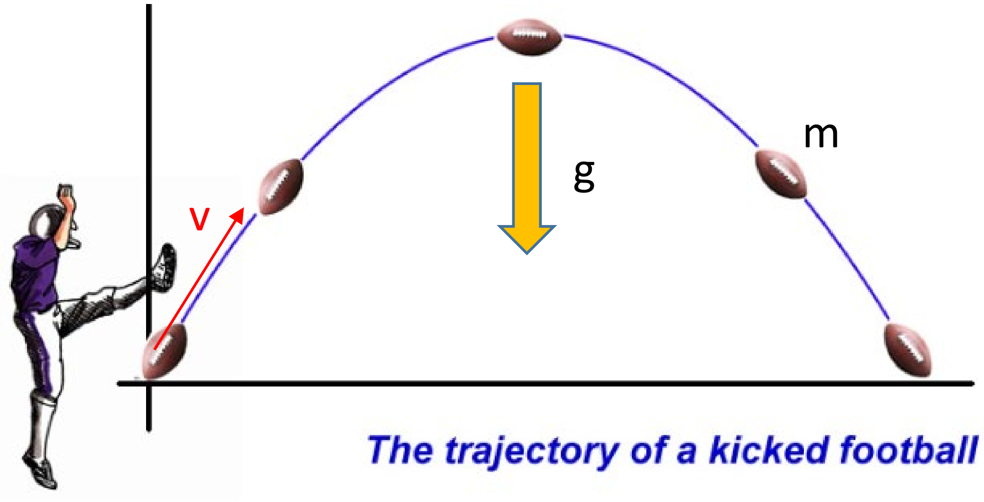
# Schrodinger's equation

In classical physics, we can work out what the trajectory (i.e. state) of the ball is using Newton's laws.

$$F = ma$$




We need an equation that tells us how a wavefunction evolves with time, like Newton's law.

Schrodinger's equation

$$i\hbar \frac{d|\psi(t)\rangle}{dt} = H|\psi(t)\rangle$$

Or this can be written equivalently as

$$\boxed{|\psi(t)\rangle = \exp(-\frac{it}{\hbar}H)|\psi(0)\rangle}$$

Given the initial state, this gives a way of calculating the state at any time later

$$|\psi(t=0)\rangle \to |\psi(t)\rangle$$

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# Breaking down Schrodinger’s Eq: Hamiltonian

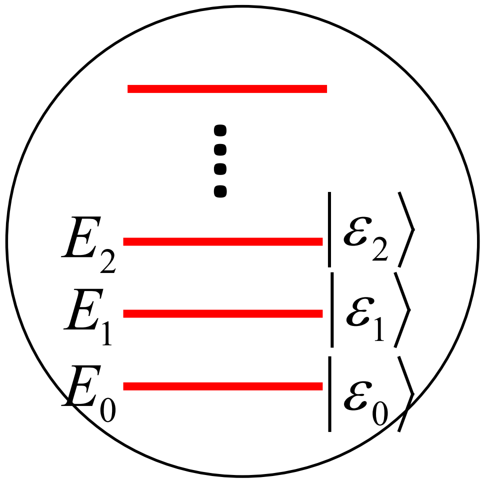
$$|\psi(t)\rangle = \exp(-\frac{it}{\hbar}H)|\psi(0)\rangle$$

$i = \sqrt{-1}$

$t =$ time (in seconds)

$\hbar = \dfrac{h}{2\pi}$ $\qquad h = 6.34 \times 10^{-34}$ Js (Planck constant)

$H =$ Hamiltonian. This is a matrix that tells us what states have what values of energy.




$$H = \sum_n E_n |\varepsilon_n\rangle\langle\varepsilon_n|$$

$$\langle\varepsilon_n|\varepsilon_m\rangle = \begin{cases} 1 & \text{if } n = m \\ 0 & \text{if } n \neq m \end{cases}$$

The energy states are orthogonal and normalized.

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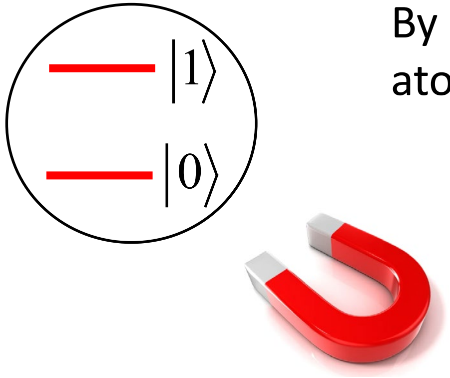
# Example: Qubit Hamiltonians

**Magnetic field on an atom**

$E_1 = B$

$E_0 = -B$




By applying a magnetic field on an atom, it is possible change the energy spacing of atoms ("Zeeman effect")

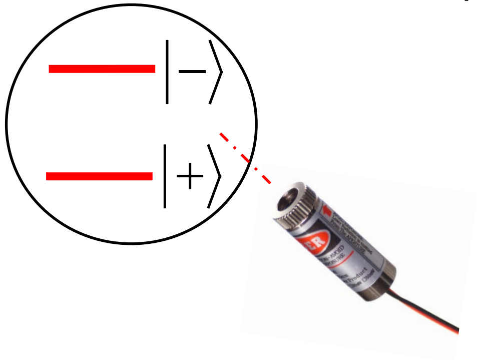
$$H = -B|0\rangle\langle 0| + B|1\rangle\langle 1| = -B\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = -BZ$$

**Laser applied to an atom**

$$H = \Omega|+\rangle\langle +| - \Omega|-\rangle\langle -| = \frac{\Omega}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} - \frac{\Omega}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} = \Omega\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \Omega X$$

$E_1 = \Omega$

$E_0 = -\Omega$

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# Matrix exponentiation

Next, the Hamiltonian is placed in the argument of the exponential

$$|\psi(t)\rangle = \boxed{\exp(-\frac{it}{\hbar}H)}|\psi(0)\rangle$$

What does it mean to exponentiate a matrix? We know that the regular exponential function can be written as an infinite series

$$e^x = 1 + x + \frac{x^2}{2} + \frac{x^3}{6} + \ldots = \sum_{n=0}^{\infty} \frac{x^n}{n!}$$

So the exponential of a matrix is defined in the same way

$$e^M = I + M + \frac{M^2}{2} + \frac{M^3}{6} + \ldots = \sum_{n=0}^{\infty} \frac{M^n}{n!}$$

The exponential of a matrix is a matrix!

Having an "i" and constants in the exponents also need to be taken to the correct power

$$e^{iM} = I + iM - \frac{M^2}{2} - \frac{iM^3}{6} + \ldots = \sum_{n=0}^{\infty} \frac{(iM)^n}{n!}$$

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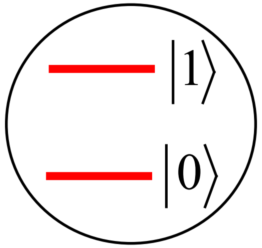
# Example 1: Magnetic field on qubit

The Hamiltonian is $$H = -BZ$$

$$E_1 = B$$
$$E_0 = -B$$




Substitute into Schrodinger's equation

$$Z^2 = I$$

$$e^{-iHt/\hbar} = I + \frac{iBt}{\hbar} Z - \frac{(Bt)^2}{2\hbar^2} I - \frac{i(Bt)^3}{6\hbar^3} Z + \ldots = \cos\frac{Bt}{\hbar} I + iZ \sin\frac{Bt}{\hbar} = \begin{pmatrix} e^{iBt/\hbar} & 0 \\ 0 & e^{-iBt/\hbar} \end{pmatrix}$$

Say initial state was

$$|\psi(0)\rangle = \alpha|0\rangle + \beta|0\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

Then the state some time later is

$$|\psi(t)\rangle = e^{-iHt/\hbar}|\psi(0)\rangle = \begin{pmatrix} e^{iBt/\hbar} & 0 \\ 0 & e^{-iBt/\hbar} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} \alpha e^{iBt/\hbar} \\ \beta e^{-iBt/\hbar} \end{pmatrix}$$

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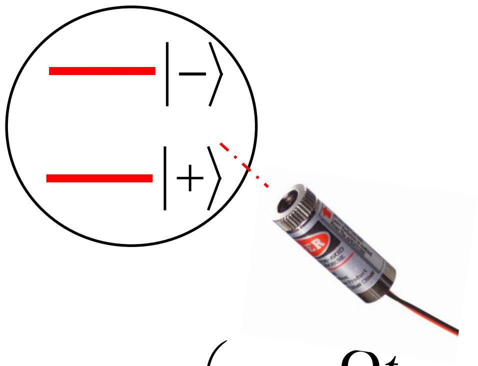
# Example 2: Laser applied to a qubit

The Hamiltonian is $H = \Omega X$

$E_1 = \Omega$

$E_0 = -\Omega$




Substitute into Schrodinger's equation

$$e^{-iHt/\hbar} = I - \frac{i\Omega t}{\hbar} X - \frac{(\Omega t)^2}{2\hbar^2} I + \frac{i(\Omega t)^3}{6\hbar^3} X + \ldots = \cos\frac{\Omega t}{\hbar} I - iX \sin\frac{\Omega t}{\hbar} = \begin{pmatrix} \cos\frac{\Omega t}{\hbar} & -i\sin\frac{\Omega t}{\hbar} \\ -i\sin\frac{\Omega t}{\hbar} & \cos\frac{\Omega t}{\hbar} \end{pmatrix}$$

$$X^2 = I$$

Say initial state was $|\psi(0)\rangle = |0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

Then the state some time later is

$$|\psi(t)\rangle = e^{-iHt/\hbar} |\psi(0)\rangle = \begin{pmatrix} \cos\frac{\Omega t}{\hbar} & -i\sin\frac{\Omega t}{\hbar} \\ -i\sin\frac{\Omega t}{\hbar} & \cos\frac{\Omega t}{\hbar} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos\frac{\Omega t}{\hbar} \\ -i\sin\frac{\Omega t}{\hbar} \end{pmatrix}$$

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# The unitary matrix

The form of the Schrodinger equation is

$$\underbrace{\boxed{|\psi(t)\rangle}}_{\text{vector}} = \underbrace{\boxed{\exp(-\frac{it}{\hbar}H)}}_{\text{matrix}} \underbrace{\boxed{|\psi(0)\rangle}}_{\text{vector}}$$

The operator (i.e. matrix) $U = \exp(-\frac{it}{\hbar}H)$ takes the state and time evolves it forward.

The Hamiltonian is a Hermitian matrix, and this makes U always a "unitary matrix"

$$U^{-1} = U^{+}$$

Generally it is not a simple task to find the explicit unitary matrix from a Hamiltonian, except in certain simple cases. Solving the Schrodinger's equation is a difficult task.

Hamiltonian=The physical process changing the state

t=The amount of time the process is applied for

U=The effect this has on the state

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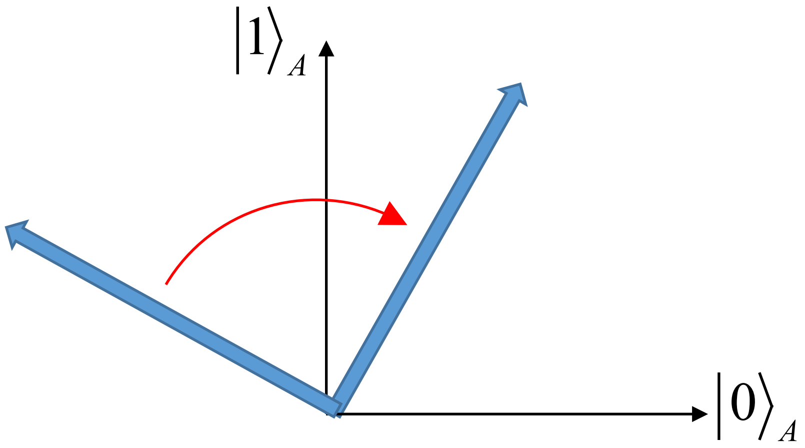
# Unitary operations as basis rotations

The name “unitary” comes from the fact that applying a unitary matrix on a vector never changes its length

$$|\psi'\rangle = U|\psi\rangle \qquad \langle\psi'|\psi'\rangle = \langle\psi|U^{+}U|\psi\rangle = \langle\psi|U^{-1}U|\psi\rangle = \langle\psi|\psi\rangle = 1$$

In fact a unitary rotation is really always just a rotation of the vector in some space




The unitary property makes means that it is always possible to reverse the  evolution of the Schrodinger equation just by applying

$$U^{+} = \exp(+\frac{it}{\hbar}H)$$

Then $$U^{+}|\psi'\rangle = U^{+}U|\psi\rangle = \exp(+\frac{it}{\hbar}H)\exp(-\frac{it}{\hbar}H)|\psi\rangle = |\psi\rangle$$

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# Question

A laser is applied on a qubit such that the Hamiltonian is $H = \Omega X$ $\Omega = 10^{-25} J$

The laser is on for t=1ns, and the initial state is prepared in

$$|\psi(0)\rangle = \frac{1}{2}|0\rangle + \frac{\sqrt{3}}{2}|1\rangle$$

What is the final state?

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# Question

A laser is applied on a qubit such that the Hamiltonian is $H = \Omega X$ $\qquad \Omega = 10^{-25} J$

The laser is on for t=1ns, and the initial state is prepared in $|\psi(0)\rangle = \frac{1}{2}|0\rangle + \frac{\sqrt{3}}{2}|1\rangle$

What is the final state?

$$|\psi(t)\rangle = e^{-iHt/\hbar}|\psi(0)\rangle = \begin{pmatrix} \cos\frac{\Omega t}{\hbar} & -i\sin\frac{\Omega t}{\hbar} \\ -i\sin\frac{\Omega t}{\hbar} & \cos\frac{\Omega t}{\hbar} \end{pmatrix} \begin{pmatrix} 1/2 \\ \sqrt{3}/2 \end{pmatrix} = \begin{pmatrix} \frac{1}{2}\cos\frac{\Omega t}{\hbar} - \frac{i\sqrt{3}}{2}\sin\frac{\Omega t}{\hbar} \\ \frac{\sqrt{3}}{2}\cos\frac{\Omega t}{\hbar} - \frac{i}{2}\sin\frac{\Omega t}{\hbar} \end{pmatrix} = \begin{pmatrix} 0.29 - 0.70i \\ 0.50 - 0.41i \end{pmatrix}$$

$$\frac{\Omega t}{\hbar} = 0.948$$

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