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Faculty of Information Technology and Bionics

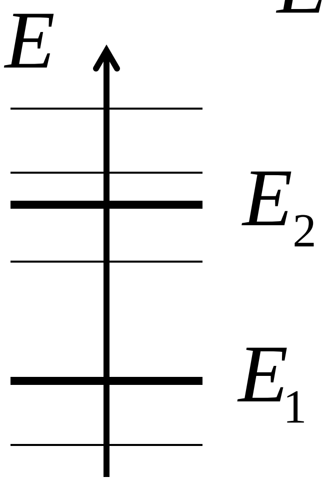
“Fides et Ratio”

Physics of Information Technology II
Physics of Molecular Bionics II
2014 Autumn

Lecture 7
Two-state atom in sinusoidal electromagnetic field
Diagonalization of a 2x2 Hermitian Matrix
General study of a two-state system
Rabi Oscillation
QuBit – Quantum Computing

Two-state atom in sinusoidal electromagnetic field

$$E_2 - E_1 \approx \hbar \cdot \omega \qquad \mathbf{E}(t) = \mathbf{E}\cos(\omega t + \varphi)$$



$$|\psi(t)\rangle = c_1(t)|1\rangle + c_2(t)|2\rangle \qquad |c_1(t)|^2 + |c_2(t)|^2 = 1$$

$$\hat{H}_0|1\rangle = E_1|1\rangle; \quad \hat{H}_0|2\rangle = E_2|2\rangle$$

$$\mathrm{j}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = \left(\hat{H}_0 + \hat{H}_I\right)|\psi(t)\rangle$$

$$\mathrm{j}\hbar\frac{\mathrm{d}c_1(t)}{\mathrm{d}t}|1\rangle + \mathrm{j}\hbar\frac{\mathrm{d}c_2(t)}{\mathrm{d}t}|2\rangle = \left(\hat{H}_0 + \hat{H}_I\right)\left[c_1(t)|1\rangle + c_2(t)|2\rangle\right]$$

$$\langle 1| \qquad \mathrm{j}\hbar\frac{\mathrm{d}c_1(t)}{\mathrm{d}t} = E_1 c_1(t) + \langle 1|\hat{H}_I|2\rangle c_2(t)$$

$$\langle 2| \qquad \mathrm{j}\hbar\frac{\mathrm{d}c_2(t)}{\mathrm{d}t} = \langle 2|\hat{H}_I|1\rangle c_1(t) + E_2 c_2(t)$$

$$\mathrm{j}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\begin{bmatrix}c_1(t)\\ c_2(t)\end{bmatrix}=\begin{bmatrix}E_1+V_{11} & \langle 1|\hat{H}_I|2\rangle\\ \langle 2|\hat{H}_I|1\rangle & E_2+V_{22}\end{bmatrix}\begin{bmatrix}c_1(t)\\ c_2(t)\end{bmatrix}$$

$$\hat{H}_I(t)=-\hat{\mathbf{D}}\cdot\mathbf{E}(t);\qquad \hat{\mathbf{D}}=q\cdot\hat{\mathbf{r}}$$

$$\langle 1|\hat{H}_I|1\rangle=\langle 1|-e\cdot\hat{\mathbf{r}}\mathbf{E}(\mathbf{r},t)|1\rangle=\int_V\phi_1^*\left[-e\mathbf{r}E(\mathbf{r}_N,t)\right]\phi_1\cdot\mathrm{d}V=V_{11}$$

$$\langle 1|\hat{H}_I|2\rangle=\langle 1|-e\cdot\hat{\mathbf{r}}\mathbf{E}(\mathbf{r},t)|2\rangle=\int_V\phi_1^*\left[-e\mathbf{r}E(\mathbf{r}_N,t)\right]\phi_2\cdot\mathrm{d}V=V_{12}$$

$$\langle 2|\hat{H}_I|1\rangle=\langle 2|-e\cdot\hat{\mathbf{r}}\mathbf{E}(\mathbf{r},t)|1\rangle=\int_V\phi_2^*\left[-e\mathbf{r}E(\mathbf{r}_N,t)\right]\phi_1\cdot\mathrm{d}V=V_{21}$$

$$\langle 1|\hat{H}_I|2\rangle=\langle 2|-e\cdot\hat{\mathbf{r}}\mathbf{E}(\mathbf{r},t)|2\rangle=\int_V\phi_2^*\left[-e\mathbf{r}E(\mathbf{r}_N,t)\right]\phi_2\cdot\mathrm{d}V=V_{22}$$

$$\mathrm{j}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\begin{bmatrix}c_1(t)\\ c_2(t)\end{bmatrix}=\begin{bmatrix}E_1+V_{11} & V_{12}\\ V_{21} & E_2+V_{22}\end{bmatrix}\begin{bmatrix}c_1(t)\\ c_2(t)\end{bmatrix}\qquad V_{12}=V_{21}^*$$

Diagonalization of a 2x2 Hermitian Matrix

$$\hat{H} = \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix}$$

H_{11}, H_{22} are real and $H_{12} = H_{21}^*$

It represents a Hermitian Operator in an orthonormal basis $\left|\varphi_1\right\rangle, \left|\varphi_2\right\rangle$

$$H_{11} + H_{22} = \mathrm{Tr}\left(\hat{H}\right)$$

Is invariant under a change in the orthonormal basis

$$\hat{H} = \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix} \equiv \begin{bmatrix} \frac{1}{2}\left(H_{11} + H_{22}\right) & 0 \\ 0 & \frac{1}{2}\left(H_{11} + H_{22}\right) \end{bmatrix} + \begin{bmatrix} \frac{1}{2}\left(H_{11} - H_{22}\right) & H_{12} \\ H_{21} & -\frac{1}{2}\left(H_{11} - H_{22}\right) \end{bmatrix}$$

$$\hat{\mathbf{H}} = \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix} \equiv \frac{1}{2}\left(H_{11} + H_{22}\right)\hat{\mathbf{1}} + \frac{1}{2}\left(H_{11} - H_{22}\right)\hat{\mathbf{K}};$$

$$\frac{1}{2}\left(H_{11} + H_{22}\right) \Rightarrow \text{Eigenvalue origin } 0$$

$$\hat{\mathbf{K}} = \begin{bmatrix} 1 & \dfrac{2H_{12}}{H_{11} - H_{22}} \\ \dfrac{2H_{21}}{H_{11} - H_{22}} & -1 \end{bmatrix}$$

$$\hat{H}\left|\psi_{\pm}\right\rangle = E_{\pm}\left|\psi_{\pm}\right\rangle \qquad E_{\pm} = \frac{1}{2}\left(H_{11}+H_{22}\right)+\frac{1}{2}\left(H_{11}-H_{22}\right)\kappa_{\pm}$$

$$\hat{K}\left|\psi_{\pm}\right\rangle = \kappa_{\pm}\left|\psi_{\pm}\right\rangle$$

Let us introduce two angles as

$$\tan\theta = \frac{2\left|H_{21}\right|}{H_{11}-H_{22}} \quad \text{with } \ 0 \le \theta < \pi$$

$$H_{21} = \left|H_{21}\right| e^{j\varphi} \qquad \text{with } \ 0 \le \varphi < 2\pi$$

$$\hat{\mathbf{K}} = \begin{bmatrix} 1 & \dfrac{2H_{12}}{H_{11}-H_{22}} \\ \dfrac{2H_{21}}{H_{11}-H_{22}} & -1 \end{bmatrix} = \begin{bmatrix} 1 & \tan\theta\cdot e^{-j\varphi} \\ \tan\theta\cdot e^{j\varphi} & -1 \end{bmatrix}$$

$$\det\left[\hat{\mathbf{K}} - \kappa\hat{\mathbf{1}}\right] = \kappa^2 - 1 - \tan^2\theta \qquad \to \kappa_{+} = +\frac{1}{\cos\theta}; \qquad \kappa_{-} = -\frac{1}{\cos\theta}$$

$$\frac{1}{\cos\theta} = \frac{\sqrt{\left(H_{11}-H_{22}\right)^2 + 4\left|H_{12}\right|^2}}{H_{11}-H_{22}}$$

$$E_{+} = \frac{1}{2}\left(H_{11}+H_{12}\right)+\frac{1}{2}\sqrt{\left(H_{11}-H_{22}\right)^2 + 4\left|H_{12}\right|^2}$$

$$E_{-} = \frac{1}{2}\left(H_{11}+H_{12}\right)-\frac{1}{2}\sqrt{\left(H_{11}-H_{22}\right)^2 + 4\left|H_{12}\right|^2}$$

Eigenvalues of $\hat{H}$

$$E_+ = \frac{1}{2}\left(H_{11} + H_{12}\right) + \frac{1}{2}\sqrt{\left(H_{11} - H_{22}\right)^2 + 4\left|H_{12}\right|^2}$$

$$E_- = \frac{1}{2}\left(H_{11} + H_{12}\right) - \frac{1}{2}\sqrt{\left(H_{11} - H_{22}\right)^2 + 4\left|H_{12}\right|^2}$$

Comments

$$E_+ + E_- = \left(H_{11} + H_{12}\right) = \mathrm{Tr}\left(\hat{H}\right)$$

$$E_+ \cdot E_- = H_{11} \cdot H_{12} - \left|H_{12}\right|^2 = \det\hat{H}$$

$$E_+ = E_- \Leftrightarrow \left(H_{11} - H_{12}\right)^2 + 4\left|H_{12}\right|^2$$

$$\rightarrow H_{11} = H_{22} \text{ and } H_{12} = H_{21} = 0$$

Normalized eigenvectors of $\hat{H}$

$$\left|\psi_+\right\rangle = \cos\frac{\theta}{2} e^{-\mathrm{j}\varphi/2}\left|\varphi_1\right\rangle + \sin\frac{\theta}{2} e^{\mathrm{j}\varphi/2}\left|\varphi_2\right\rangle$$

$$\left|\psi_-\right\rangle = -\sin\frac{\theta}{2} e^{-\mathrm{j}\varphi/2}\left|\varphi_1\right\rangle + \cos\frac{\theta}{2} e^{\mathrm{j}\varphi/2}\left|\varphi_2\right\rangle$$

$$\left\langle\psi_+ \middle| \psi_-\right\rangle = 0$$

$$\left\langle\psi_+ \middle| \psi_+\right\rangle = 1$$

$$\left\langle\psi_- \middle| \psi_-\right\rangle = 1$$

General study of a two-state system

$$\hat{H}_0 \left| \varphi_1 \right\rangle = E_1 \left| \varphi_1 \right\rangle; \quad \hat{H}_0 \left| \varphi_2 \right\rangle = E_2 \left| \varphi_2 \right\rangle \qquad \left\langle \varphi_i \middle| \varphi_j \right\rangle = \delta_{ij} \quad i, j = 1, 2$$

$$\hat{H} = \hat{H}_0 + \hat{W}$$

$$\hat{H} \left| \psi_+ \right\rangle = E_+ \left| \psi_+ \right\rangle; \quad \hat{H} \left| \psi_- \right\rangle = E_- \left| \psi_- \right\rangle$$

$$\hat{W} = \begin{bmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{bmatrix} \qquad W_{11}, W_{22} \text{ are real and } W_{12} = W_{21}^*$$

Consequences of the interaction (coupling, perturbation)

E_1 and E_2 are no longer the possible energies of the system

$\left| \varphi_1 \right\rangle$ and $\left| \varphi_2 \right\rangle$ are no longer stationary states

Static Aspect: Effect of Interaction on the Stationary States

Eigen-states and eigen-values

In the $|\varphi_1\rangle$, $|\varphi_2\rangle$ basis the matrix representing the system

$$\hat{H} = \hat{H}_0 + \hat{W} = \begin{bmatrix} E_1 + W_{11} & W_{12} \\ W_{21} & E_2 + W_{22} \end{bmatrix}$$

Diagonalization

$$E_+ = \frac{1}{2}\left(E_1 + W_{11} + E_2 + W_{22}\right) + \frac{1}{2}\sqrt{\left(E_1 + W_{11} - E_2 - W_{22}\right)^2 + 4\left|W_{12}\right|^2}$$

$$E_- = \frac{1}{2}\left(E_1 + W_{11} + E_2 + W_{22}\right) - \frac{1}{2}\sqrt{\left(E_1 + W_{11} - E_2 - W_{22}\right)^2 + 4\left|W_{12}\right|^2}$$

$$\tan\theta = \frac{2\left|W_{21}\right|}{E_1 + W_{11} - E_2 - W_{22}} \quad \text{with } 0 \le \theta < \pi; \quad W_{21} = \left|W_{21}\right| e^{\mathrm{j}\varphi} \qquad \text{with } 0 \le \varphi < 2\pi$$

$$\left|\psi_+\right\rangle = \cos\frac{\theta}{2} e^{-\mathrm{j}\varphi/2}\left|\varphi_1\right\rangle + \sin\frac{\theta}{2} e^{\mathrm{j}\varphi/2}\left|\varphi_2\right\rangle$$

$$\left|\psi_-\right\rangle = -\sin\frac{\theta}{2} e^{-\mathrm{j}\varphi/2}\left|\varphi_1\right\rangle + \cos\frac{\theta}{2} e^{\mathrm{j}\varphi/2}\left|\varphi_2\right\rangle$$

Dynamical Aspect: Oscillation between two Unperturbed States

$$\left|\psi(t)\right\rangle = c_1(t)\left|1\right\rangle + c_2(t)\left|2\right\rangle$$

$$\mathrm{j}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\left|\psi(t)\right\rangle = \left(\hat{H}_0 + \hat{W}\right)\left|\psi(t)\right\rangle \qquad W_{11} = W_{22} = 0$$

$$\mathrm{j}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\begin{bmatrix} c_1(t) \\ c_2(t) \end{bmatrix} = \begin{bmatrix} E_1 & W_{12} \\ W_{21} & E_2 \end{bmatrix}\begin{bmatrix} c_1(t) \\ c_2(t) \end{bmatrix} \qquad \left|\psi_+\right\rangle, E_+ \quad \left|\psi_-\right\rangle, E_-$$

$$\left|\psi(0)\right\rangle = \lambda\left|\psi_+\right\rangle + \mu\left|\psi_-\right\rangle \qquad \left|\psi(t)\right\rangle = \lambda e^{-\mathrm{j}\frac{E_+}{\hbar}t}\left|\psi_+\right\rangle \mu e^{-\mathrm{j}\frac{E_-}{\hbar}t}\left|\psi_-\right\rangle$$

This enables us to obtain $c_1(t)$ and $c_2(t)$ by projecting $\left|\psi(t)\right\rangle$

onto $\left|1\right\rangle$ and $\left|2\right\rangle$

The system oscillates between the two unperturbed states

$$\left|1\right\rangle \text{ and } \left|2\right\rangle$$

Let the system be in $\left|1\right\rangle$ at t = 0. $\left|\psi(0)\right\rangle = \left|1\right\rangle$

Calculate the probability of finding the system in state $\left|2\right\rangle$ at time t

Let us expand the initial state on the $\left|\psi_{+}\right\rangle, \left|\psi_{-}\right\rangle$ basis

$$\left|\psi(0)\right\rangle = \left|1\right\rangle = e^{\mathrm{j}\varphi/2}\left[\cos\frac{\theta}{2}\left|\psi_{+}\right\rangle - \sin\frac{\theta}{2}\left|\psi_{-}\right\rangle\right]$$

$$\left|\psi(t)\right\rangle = e^{\mathrm{j}\varphi/2}\left[\cos\frac{\theta}{2}e^{-\mathrm{j}\frac{E_{+}}{\hbar}t}\left|\psi_{+}\right\rangle - \sin\frac{\theta}{2}e^{-\mathrm{j}\frac{E_{-}}{\hbar}t}\left|\psi_{-}\right\rangle\right]$$

The probability amplitude of finding the system at t in the state $\left|2\right\rangle$

$$\left\langle 2\middle|\psi(t)\right\rangle = e^{\mathrm{j}\varphi/2}\left[\cos\frac{\theta}{2}e^{-\mathrm{j}\frac{E_{+}}{\hbar}t}\left\langle 2\middle|\psi_{+}\right\rangle - \sin\frac{\theta}{2}e^{-\mathrm{j}\frac{E_{-}}{\hbar}t}\left\langle 2\middle|\psi_{-}\right\rangle\right] =$$

$$= e^{\mathrm{j}\varphi}\sin\frac{\theta}{2}\cos\frac{\theta}{2}\left[e^{-\mathrm{j}\frac{E_{+}}{\hbar}t} - e^{-\mathrm{j}\frac{E_{-}}{\hbar}t}\right]$$

$$P_{12}(t) = \left| \langle 2 | \psi(t) \rangle \right|^2 = \sin^2\theta \cdot \sin^2\left(\frac{E_+ - E_-}{\hbar} t \right)$$

$$P_{12}(t) = \frac{4|W_{12}|^2}{4|W_{12}|^2 + (E_1 - E_2)^2} \sin^2\left[\sqrt{4|W_{12}|^2 + (E_1 - E_2)^2} \, \frac{t}{2\hbar} \right]$$

Rabi formula – Rabi Oscillation

(Isaak Rabi, Nobel Prize 1944)

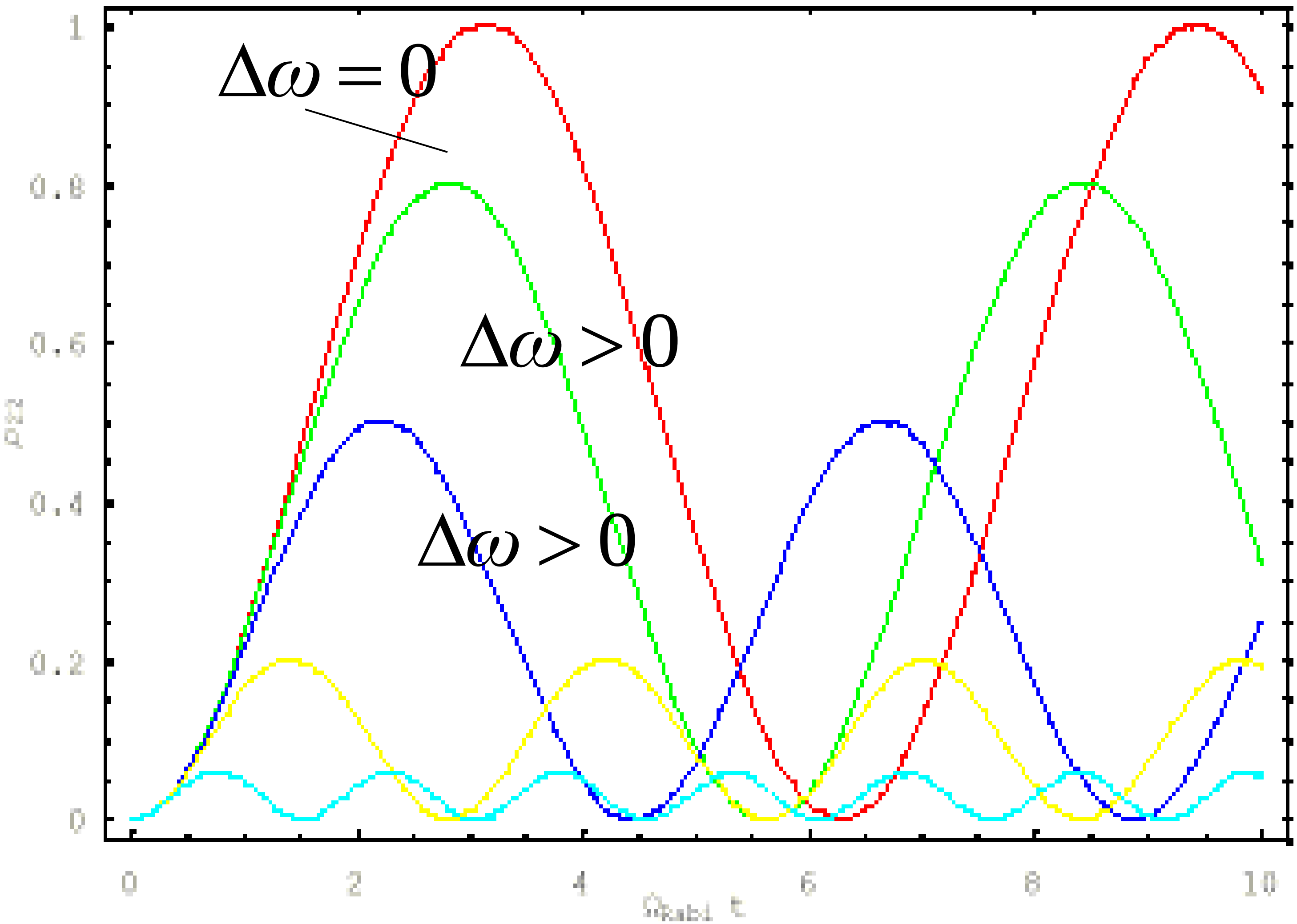
$P_{12}(t)$ Oscillates over time with a frequency of $\Omega_{Rabi} = \left(\frac{E_+ - E_-}{\hbar} \right)$

$$\Delta\omega = \omega_{21} - \omega \qquad \eta = 2\frac{V_{21}E_0}{\hbar}$$

$$\Omega = \sqrt{\eta^2 + (\Delta\omega)^2}$$

$$P_1 = \cos^2\frac{1}{2}\Omega\, t + \left(\frac{\Delta\omega}{\Omega}\right)^2 \sin^2\frac{1}{2}\Omega\, t$$

$$P_2 = \left(\frac{\eta}{\Omega}\right)^2 \sin^2\frac{1}{2}\Omega\, t$$



$\Delta\omega = 0$
$\Delta\omega > 0$
$\Delta\omega > 0$
1
0.8
0.6
0.4
0.2
0
0
2
4
6
8
10

Rabi Oscillations:

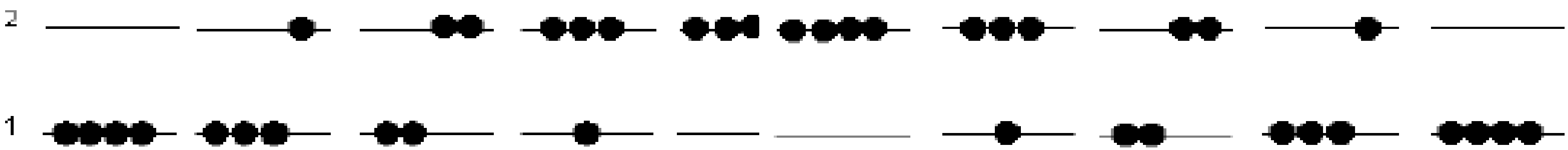
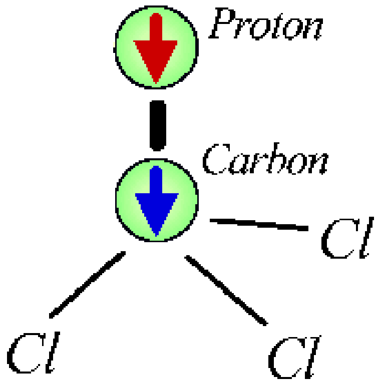
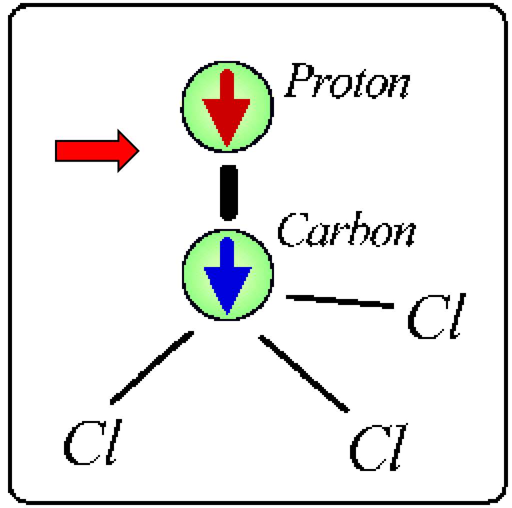
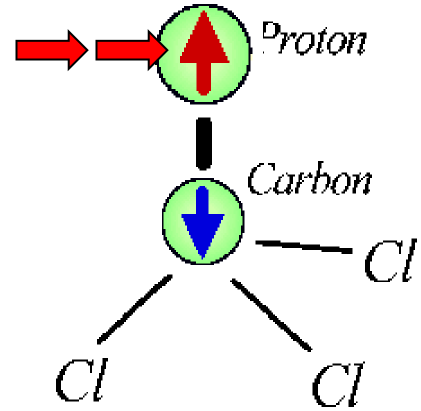


Figure 1.1. *Evolution of the two-level atom with continuous sinusoidal radiation incident upon it – The Rabi atom. Population moves from one level to another until all atoms are in the excited state and then back again. With passing time this pattern repeats sinusoidally.*







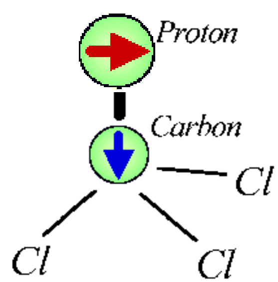
$$|0\rangle, |0\rangle$$

$$|0\rangle\,|0\rangle$$

$$|0\rangle, |1\rangle$$

$$\frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)$$

Pure entangled state

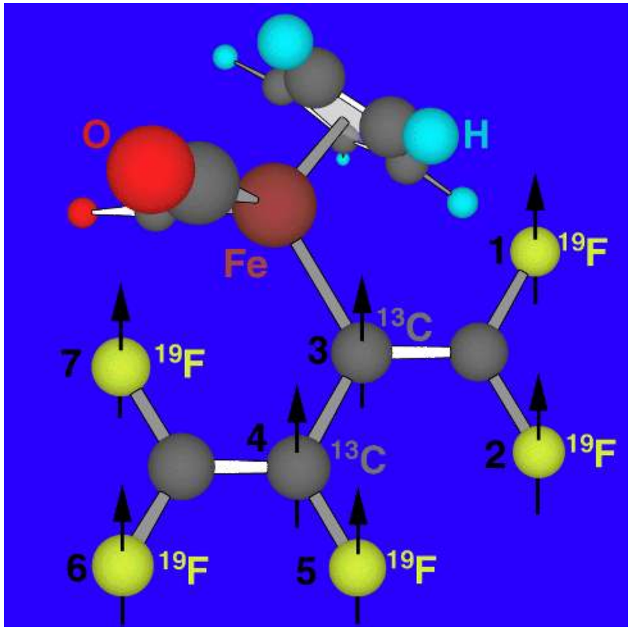


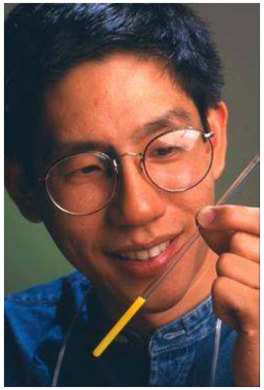
$$\frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)$$

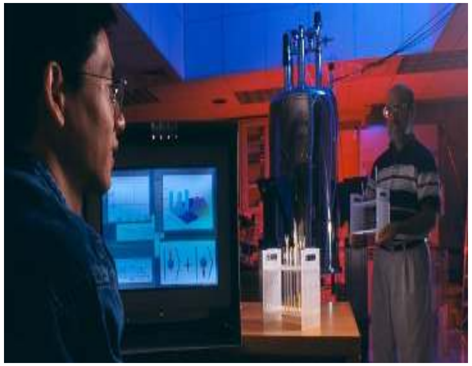
NMR Quantum Computers

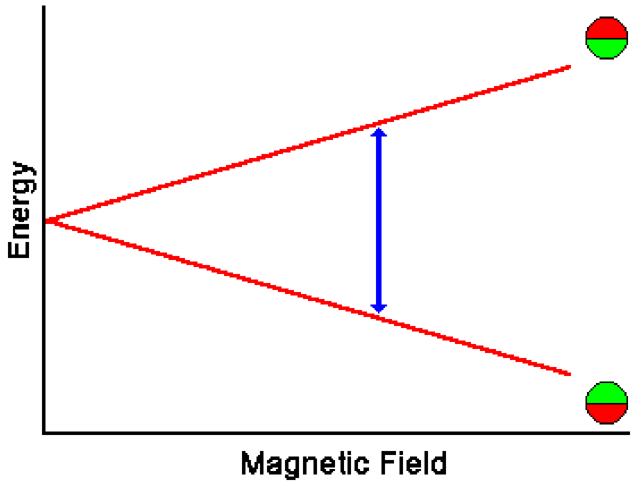
A nearly ideal physical system that can be used as quantum computer is a single molecule, in which nuclear spins of individual atoms represent “qu-bits”.

IBM’s 7 qubit -Quantum Computer



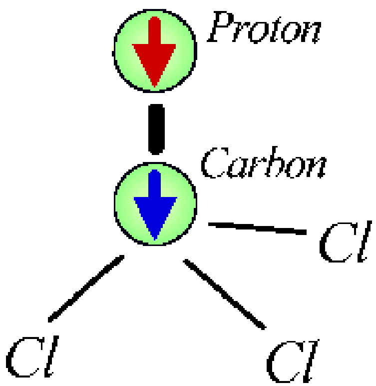




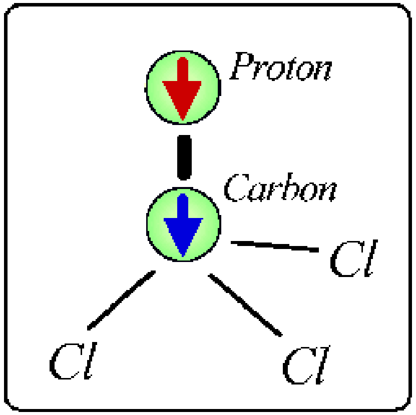


Using nuclear magnetic resonance (NMR) techniques,
the spins can be manipulated, initialized and measured.

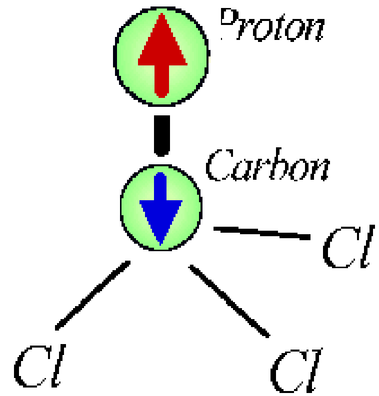
The quantum behavior of the spins can be exploited to perform quantum computation; for example, the carbon and hydrogen nuclei in a chloroform molecule represent two qubits.



$$|0\rangle, |0\rangle$$



$$|0\rangle |0\rangle$$



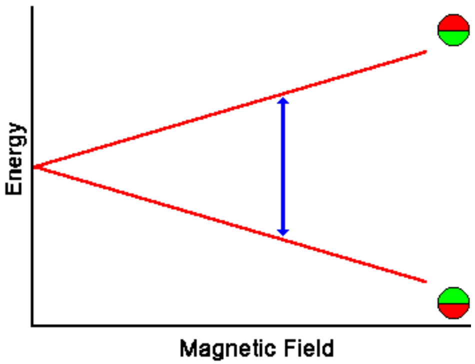
$$|0\rangle, |1\rangle$$

Applying a radio-frequency pulse to the hydrogen nucleus addresses that qubit, and causes it to rotate from a |0> state to a superposition state.

Register : Multispin state : $\Psi = |00101011\ldots\rangle$

Put the spins in a strong enough magnetic field,

and then let them cool down. $\Psi = |0000000\ldots\rangle$



Illuminate the spins with radiation that is tuned to the resonant frequency connecting the lower, spin-down state with the upper spin-up state.

Assuming that only one of the spins is in resonance, it will switch.

Using nuclear magnetic resonance (NMR) techniques, these spins can be manipulated, initialized and measured.

A nearly ideal physical system that can be used as quantum computer is a single molecule, in which nuclear spins of individual atoms represent “qubits”.