#### Lecture 18

## **Light-Matter Interaction and Optical Transitions - I**

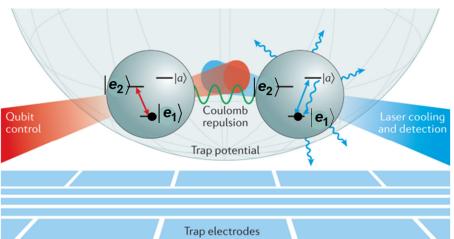
#### In this lecture you will learn:

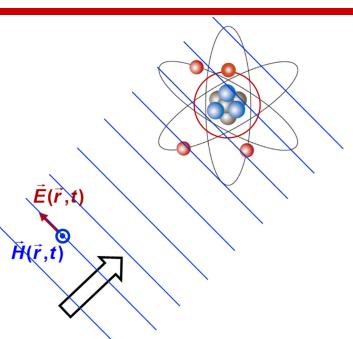
#### Part I:

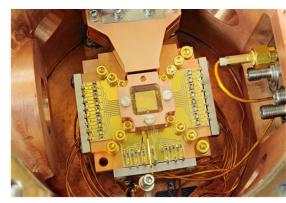
- Classical electrodynamics
- Gauge transformations
- Light-matter interaction Hamiltonian

#### Part II:

- Electric-dipole Hamiltonian
- Transformation to a spin Hamiltonian
- Rabi oscillations







An ion-trap chip, NIST (2011)

## **Light-Matter Interaction**

• Part I (for the self-reading of graduate students)

Classical and quantum physics of charged particles

Derivation of the electric-dipole Hamiltonian for light-matter interaction

Part II

Interaction of a TLS (an electron in an atom) with light

# Part

## **Quantum Commutation Relations: A Recap**

In quantum mechanics we have for a particle:

$$\left[\hat{\mathbf{r}}_{\mathbf{k}},\hat{\boldsymbol{\rho}}_{j}\right]=i\hbar\delta_{\mathbf{k}j}$$

This implies:

$$\hat{\vec{p}} = m\hat{\vec{v}} \iff \frac{\hbar}{i}\nabla \longrightarrow \text{Kinetic momentum}$$
of the particle
$$\left\langle \vec{r} \, \middle| \, \hat{\vec{p}} \middle| \psi(t) \right\rangle = \frac{\hbar}{i}\nabla\psi(\vec{r}, t)$$

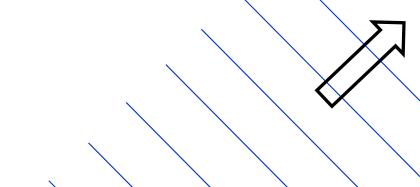
Kinetic energy of the particle in free-space:

$$\hat{H} = \frac{\hat{\vec{p}}.\hat{\vec{p}}}{2m} = \frac{\hat{p}^2}{2m}$$

But what if the particle is charged? Do the above hold?

## Classical Electrodynamics (Nothing to do with Quantum Physics)

Consider an electromagnetic wave travelling in free space:



**Electromagnetic wave energy is:** 

$$\int d^3\vec{r} \left\{ \frac{1}{2} \, \varepsilon_{\rm o} \, \vec{E}(\vec{r},t) . \vec{E}(\vec{r},t) + \frac{1}{2} \, \mu_{\rm o} \vec{H}(\vec{r},t) . \vec{H}(\vec{r},t) \right\}$$

**Electromagnetic wave momentum is:** 

$$\varepsilon_{o}\mu_{o}\int d^{3}\vec{r}\ \vec{E}(\vec{r},t)\times\vec{H}(\vec{r},t)$$

The electric and magnetic fields can be represented by scalar and vector potentials:

$$\vec{E}(\vec{r},t) = -\frac{\partial \vec{A}(\vec{r},t)}{\partial t} - \nabla \phi(\vec{r},t)$$

$$\vec{H}(\vec{r},t) = \frac{1}{\mu_{o}} \nabla \times \vec{A}(\vec{r},t)$$

The vector and scalar potential description is <u>redundant</u> (we are representing 3 degrees of freedom with 4 degrees of freedom)

This means the description of electric and magnetic fields in terms of vector and scalar potentials cannot be unique!

## Gauge Transformations and Non-Uniqueness of Electromagnetic Potentials

Suppose one had figured out the vector and scalar potentials such that:

$$\vec{E}(\vec{r},t) = -\frac{\partial \vec{A}(\vec{r},t)}{\partial t} - \nabla \phi(\vec{r},t)$$

$$\vec{H}(\vec{r},t) = \frac{1}{\mu_0} \nabla \times \vec{A}(\vec{r},t)$$

Suppose, amid calculations, one decides to change the vector and scalar potentials as follows:

$$\vec{A}_{new}(\vec{r},t) = \vec{A}(\vec{r},t) + \nabla F(\vec{r},t)$$

$$\phi_{new}(\vec{r},t) = \phi(\vec{r},t) - \frac{\partial}{\partial t}F(\vec{r},t)$$

$$F(\vec{r},t) \text{ is any scalar function}$$

One would still get the same physical electric and magnetic fields:

$$\vec{E}(\vec{r},t) = -\frac{\partial \vec{A}_{new}(\vec{r},t)}{\partial t} - \nabla \phi_{new}(\vec{r},t)$$

$$\vec{H}(\vec{r},t) = \frac{1}{\mu_{o}} \nabla \times \vec{A}_{new}(\vec{r},t)$$

Scalar and vector potentials are not unique (they depend on the choice of gauge)! But physical measurable quantities should not depend on the choice of gauge

## **Classical Electrodynamics and Gauge Choice**

The vector and scalar potential description is <u>redundant</u> (we are representing 3 degrees of freedom with 4 degrees of freedom)

We can tie up the extra degree of freedom by a assuming an arbitrary relation between  $\vec{A}(\vec{r},t)$  and  $\phi(\vec{r},t)$  called the gauge condition:

#### **Coulomb Gauge:**

$$\nabla . \vec{A}(\vec{r},t) = 0$$
 We will choose this gauge

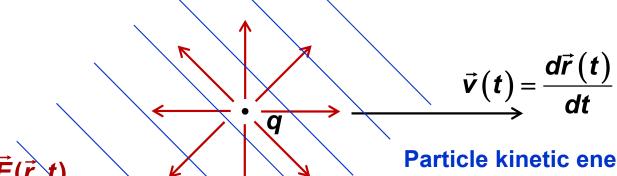
#### **Lorentz Gauge:**

$$\nabla . \vec{A}(\vec{r},t) + \frac{1}{c^2} \frac{\partial \phi(\vec{r},t)}{\partial t} = 0$$

**Another Possible Gauge Choice:** 

$$\phi(\vec{r},t)=0$$

Now consider a charged particle (charge = q) in an electromagnetic wave:



Particle kinetic energy is:

$$\frac{1}{2}m\vec{v}(t).\vec{v}(t)$$

**Electromagnetic wave energy is:** 

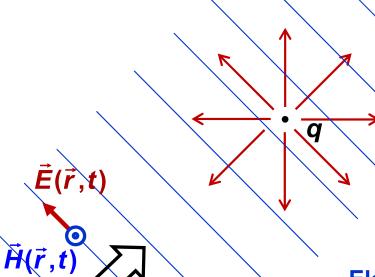
$$\int d^3\vec{r} \left\{ \frac{1}{2} \, \varepsilon_{\rm o} \, \vec{E}(\vec{r},t) . \vec{E}(\vec{r},t) + \frac{1}{2} \, \mu_{\rm o} \vec{H}(\vec{r},t) . \vec{H}(\vec{r},t) \right\}$$

Total energy of the particle-field system is:

$$E_{total} = \frac{1}{2}m\vec{v}(t).\vec{v}(t) + q\phi(\vec{r}(t),t) + \int d^3\vec{r} \left\{ \frac{1}{2} \varepsilon_o \vec{E}(\vec{r},t).\vec{E}(\vec{r},t) + \frac{1}{2} \mu_o \vec{H}(\vec{r},t).\vec{H}(\vec{r},t) \right\}$$

Easy peasy !!

Again consider a charged particle (charge = q) in an electromagnetic wave:



$$\overrightarrow{v}(t) = \frac{d\overrightarrow{r}(t)}{dt}$$

Particle kinetic momentum is:

$$m\vec{v}(t) = m\frac{d\vec{r}(t)}{dt}$$

**Electromagnetic wave momentum is:** 

$$\varepsilon_{o}\mu_{o}\int d^{3}\vec{r}\ \vec{E}(\vec{r},t)\times\vec{H}(\vec{r},t)$$

Total momentum of the particle-field system is:

$$\vec{p}_{total}(t) = m \frac{d\vec{r}(t)}{dt} + q\vec{A}(\vec{r}(t),t) + \varepsilon_{o}\mu_{o} \int d^{3}\vec{r} \ \vec{E}(\vec{r},t) \times \vec{H}(\vec{r},t)$$

Kinetic momentum of the particle



**Electromagnetic** momentum of the wave

$$\vec{p}_{total}(t) = m \frac{d\vec{r}(t)}{dt} + q \vec{A}(\vec{r}(t),t) + \varepsilon_o \mu_o \int d^3 \vec{r} \ \vec{E}(\vec{r},t) \times \vec{H}(\vec{r},t)$$

Kinetic momentum of the particle

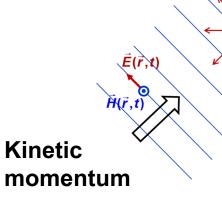


Electromagnetic momentum of the wave

Define a canonical momentum of the particle as:

$$\vec{p}(t) = m\vec{v}(t) + q\vec{A}(\vec{r}(t),t)$$

$$\Rightarrow m\vec{v}(t) = \vec{p}(t) - q\vec{A}(\vec{r}(t),t)$$
 ———



Particle kinetic energy is:

$$\frac{1}{2}m\vec{v}(t).\vec{v}(t) = \frac{\left[\vec{p}(t) - q\vec{A}(\vec{r}(t),t)\right]^2}{2m}$$

Total particle energy (kinetic + potential) is:

$$H = \frac{1}{2}m\vec{v}(t).\vec{v}(t) + q\phi(\vec{r}(t),t) = \frac{\left[\vec{p}(t) - q\vec{A}(\vec{r}(t),t)\right]^{2}}{2m} + q\phi(\vec{r}(t),t)$$

#### **Quantum Commutation Relations**

#### We have:

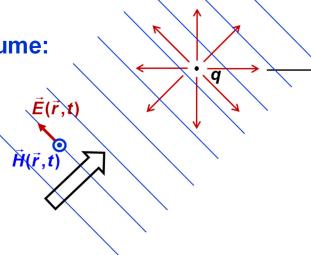
$$\vec{p}(t) = m\vec{v}(t) + q\vec{A}(\vec{r}(t),t)$$

In imposing commutation relations, should we assume:

$$\begin{bmatrix} \hat{r}_{k}, m\hat{v}_{j} \end{bmatrix} = i\hbar\delta_{kj}$$
Kinetic
momentum

Or, should we assume:

$$\begin{bmatrix} \hat{r}_{k}, \hat{p}_{j} \end{bmatrix} = i\hbar \delta_{kj}$$
Canonical momentum



### Turns out only the latter works!

$$\begin{bmatrix} \hat{r}_{k}, \hat{p}_{j} \end{bmatrix} = i\hbar \delta_{kj} \qquad \begin{bmatrix} \hat{p}_{k}, \hat{p}_{j} \end{bmatrix} = 0 \qquad \begin{bmatrix} \hat{r}_{k}, \hat{r}_{j} \end{bmatrix} = 0$$

$$\Rightarrow \langle \vec{r} | \hat{\vec{p}} | \psi(t) \rangle = \frac{\hbar}{i} \nabla \psi(\vec{r}, t)$$

$$i\hbar q \varepsilon_{kjs} \mu_{o} H_{s}(\hat{r}, t)$$

$$\varepsilon_{123} = 1$$
 (fully antisymmetric)

e.g.: 
$$\varepsilon_{123} = 1, \varepsilon_{132} = -1, \varepsilon_{312} = 1, \dots$$

$$\begin{bmatrix} m\hat{v}_k, m\hat{v}_j \end{bmatrix} = i\hbar q \varepsilon_{kjs} \mu_0 H_s(\hat{r}, t)$$
Levi-Civita symbol

## **Time-Dependent Quantum Hamiltonian**

Total classical particle energy (kinetic + potential) is:

$$H = \frac{1}{2}m\vec{v}(t).\vec{v}(t) + q\phi(\vec{r}(t),t) = \frac{\left[\vec{p}(t) - q\vec{A}(\vec{r}(t),t)\right]^{2}}{2m} + q\phi(\vec{r}(t),t)$$

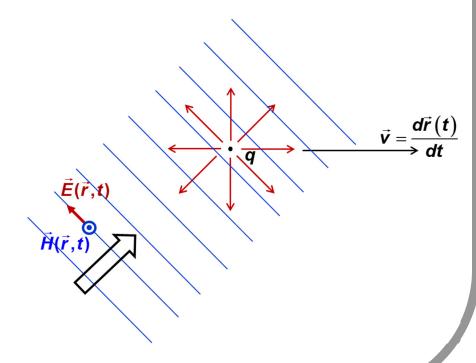
The quantum Hamiltonian operator becomes:

$$\hat{H}(t) = \frac{1}{2}m\hat{\vec{v}}.\hat{\vec{v}} + q\phi(\hat{\vec{r}},t) = \frac{\left[\hat{\vec{p}} - q\hat{A}(\hat{\vec{r}},t)\right]^2}{2m} + q\phi(\hat{\vec{r}},t)$$

The Hamiltonian operator is <u>time-dependent!</u>

We will now need to solve the time-dependent Schrödinger equation:

$$i\hbar \frac{\partial \left|\psi(t)\right\rangle}{\partial t} = \hat{H}(t)\left|\psi(t)\right\rangle$$



## **Time-Dependent Schrödinger Equation**

We have:

$$i\hbar \frac{\partial \left| \psi(t) \right\rangle}{\partial t} = \hat{H}(t) \left| \psi(t) \right\rangle$$

Where:

$$\hat{H}(t) = \frac{\left[\hat{\vec{p}} - q\vec{A}(\hat{\vec{r}},t)\right]^2}{2m} + q\phi(\hat{\vec{r}},t)$$

$$\begin{bmatrix}
\hat{r}_{k}, \hat{\rho}_{j} \end{bmatrix} = i\hbar \delta_{kj} \\
\Rightarrow \langle \vec{r} | \hat{\vec{p}} | \psi(t) \rangle = \frac{\hbar}{i} \nabla \psi(\vec{r}, t)$$

It follows that:

$$i\hbar \frac{\partial \langle \vec{r} | \psi(t) \rangle}{\partial t} = \langle \vec{r} | \hat{H}(t) | \psi(t) \rangle$$

$$\Rightarrow i\hbar \frac{\partial \psi(\vec{r}, t)}{\partial t} = \langle \vec{r} | \frac{\left[ \hat{\vec{p}} - q\vec{A} (\hat{\vec{r}}, t) \right]^{2}}{2m} + q\phi(\hat{\vec{r}}, t) | \psi(t) \rangle$$

$$\Rightarrow i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t} = \frac{\left[\frac{\hbar}{i}\nabla - q\vec{A}(\vec{r},t)\right]^2}{2m} \psi(\vec{r},t) + q\phi(\hat{\vec{r}},t)\psi(\vec{r},t)$$

But wait a minute ..... the vector and scalar potentials are not unique and are gauge-dependent!!

So how can the above Schrodinger equation be universally correct ??

## **Quantum States and Gauge Choice**

$$i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t} = \frac{\left[\frac{\hbar}{i}\nabla - q\vec{A}(\vec{r},t)\right]^2}{2m} \psi(\vec{r},t) + q\phi(\hat{r},t)\psi(\vec{r},t)$$

Suppose we make a gauge transformation (in our heads):

$$\vec{A}_{new}(\vec{r},t) = \vec{A}(\vec{r},t) + \nabla F(\vec{r},t)$$

$$\phi_{new}(\vec{r},t) = \phi(\vec{r},t) - \frac{\partial}{\partial t}F(\vec{r},t)$$

$$F(\vec{r},t) \text{ is a scalar function}$$

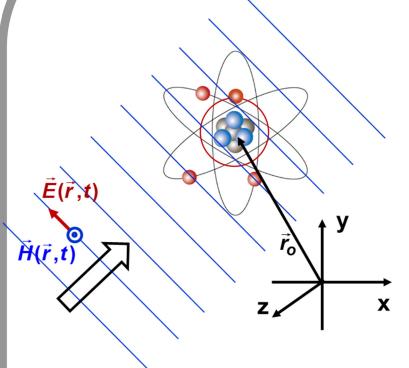
And if we also assume that under this gauge transformation:

$$\psi_{new}(\vec{r},t) = e^{i\frac{q}{\hbar}F(\vec{r},t)}\psi(\vec{r},t)$$
  $|\psi_{new}(t)\rangle = e^{i\frac{q}{\hbar}F(\hat{r},t)}|\psi(t)\rangle$ 

Then we get (after substituting the above in the Schrodinger equation at the top):

$$i\hbar \frac{\partial \psi_{new}(\vec{r},t)}{\partial t} = \frac{\left[\frac{\hbar}{i}\nabla - q\vec{A}_{new}(\vec{r},t)\right]^{2}}{2m}\psi_{new}(\vec{r},t) + q\phi_{new}(\hat{\vec{r}},t)\psi_{new}(\vec{r},t)$$

- Quantum states and quantum wavefunctions are gauge dependent!
- But the form of the Schrodinger equation is gauge independent!
- The probability density  $\left|\psi(ec{r},t)
  ight|^2$  is also gauge independent !



$$i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t} = \frac{\left[\frac{\hbar}{i}\nabla - q\vec{A}(\vec{r},t)\right]^2}{2m} \psi(\vec{r},t) + q\phi(\hat{\vec{r}},t)\psi(\vec{r},t) + V(\vec{r})\psi(\vec{r},t)$$
Scalar potential of the wave

Coulomb Gauge:  $\nabla . \vec{A}(\vec{r},t) = 0$ 

$$\vec{E}(\vec{r},t) = -\frac{\partial \vec{A}(\vec{r},t)}{\partial t} - \nabla \phi(\vec{r},t)$$

$$\nabla \cdot \vec{E}(\vec{r},t) = 0 \Rightarrow -\nabla^2 \phi(\vec{r},t) = 0$$

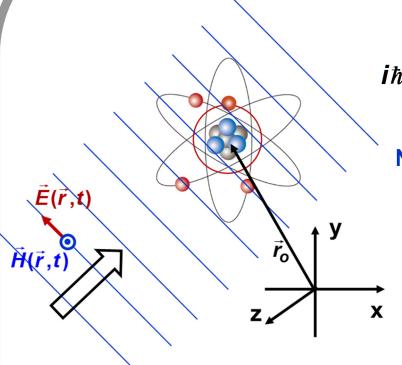
$$\Rightarrow \phi(\vec{r},t) = 0$$

#### So we have:

$$\vec{E}(\vec{r},t) = -\frac{\partial \vec{A}(\vec{r},t)}{\partial t}$$

$$\vec{H}(\vec{r},t) = \frac{1}{u_0} \nabla \times \vec{A}(\vec{r},t)$$

$$i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t} = \frac{\left[\frac{\hbar}{i}\nabla - q\vec{A}(\vec{r},t)\right]^2}{2m} \psi(\vec{r},t) + V(\vec{r})\psi(\vec{r},t)$$



$$i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} = \frac{\left[\frac{\hbar}{i}\nabla - q\vec{A}(\vec{r},t)\right]^2}{2m}\psi(\vec{r},t) + V(\vec{r})\psi(\vec{r},t)$$

Now:

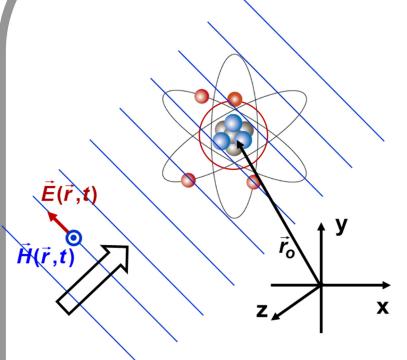
$$\vec{A}(\vec{r},t) = A_0 \cos(\vec{k}\cdot\vec{r} - \omega t)$$

Assume that the potential well (atom) is located at  $\vec{r} = \vec{r}_0$  then at the location of the atom:

$$\vec{A}(\vec{r},t) \approx \vec{A}(\vec{r}_o,t) = A_o \cos(\vec{k}.\vec{r}_o - \omega t)$$

Then we can approximate the Schrodinger equation as (because the field is pretty much uniform in space as far as the atom is concerned):

$$i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t} = \frac{\left[\frac{\hbar}{i}\nabla - q\vec{A}(\vec{r}_{o},t)\right]^{2}}{2m}\psi(\vec{r},t) + V(\vec{r})\psi(\vec{r},t)$$



$$i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t} = \frac{\left[\frac{\hbar}{i}\nabla - q\vec{A}(\vec{r}_{o},t)\right]^{2}}{2m}\psi(\vec{r},t)$$
$$+V(\vec{r})\psi(\vec{r},t)$$

#### Now do a gauge transformation:

$$\vec{A}_{new}(\vec{r},t) = \vec{A}(\vec{r},t) + \nabla F(\vec{r},t)$$

$$\phi_{new}(\vec{r},t) = \phi(\vec{r},t) - \frac{\partial}{\partial t}F(\vec{r},t)$$

$$\psi_{new}(\vec{r},t) = e^{i\frac{q}{\hbar}F(\vec{r},t)}\psi(\vec{r},t)$$

#### **Choose:**

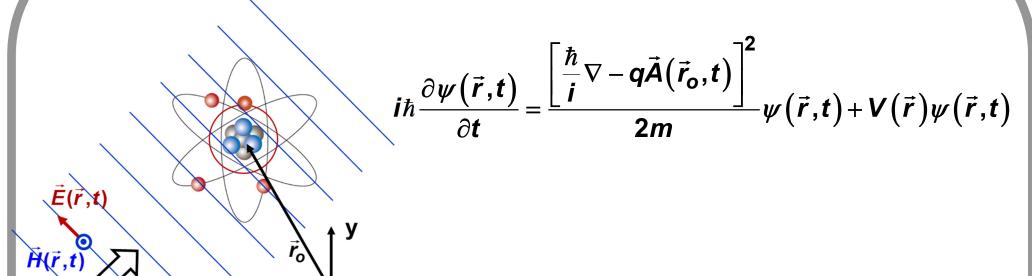
$$F(\vec{r},t) = -\vec{A}(\vec{r}_{o},t). \vec{r}$$
  $\Rightarrow$   $\nabla F(\vec{r},t) = -\vec{A}(\vec{r}_{o},t)$ 

$$\nabla F(\vec{r},t) = -\vec{A}(\vec{r}_{o},t)$$

#### Which gives:

$$\vec{A}_{new}(\vec{r}_o,t)=0$$

$$\phi_{\text{new}}(\vec{r}_{\text{o}},t) = \phi(\vec{r}_{\text{o}},t) + \frac{\partial}{\partial t}\vec{A}(\vec{r}_{\text{o}},t).\vec{r} = -\vec{E}(\vec{r}_{\text{o}},t).\vec{r}$$



After the gauge transformation we get:

$$i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t} = \frac{\left[\frac{\hbar}{i}\nabla\right]^2}{2m} \psi(\vec{r},t) + \left[V(\vec{r}) - q\vec{E}(\vec{r}_0,t).\vec{r}\right] \psi(\vec{r},t)$$

The particle Hamiltonian is effectively:

$$\hat{H}(t) = \frac{\hat{p}^2}{2m} + V(\hat{r}) - q\vec{E}(\vec{r}_o, t).\vec{r}$$

## Part II

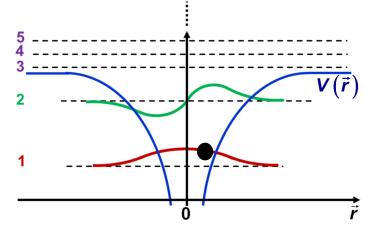
## Particle in a Potential Well (an Atom)

Suppose the Hamiltonian of a confined particle inside some potential is:

$$\hat{H}_{o} = \frac{\hat{p}^2}{2m} + V(\vec{r})$$

Let the energy eigenstates be defined as:

$$\hat{H}_{o}\left|\mathbf{e}_{j}\right\rangle = E_{j}\left|\mathbf{e}_{j}\right\rangle$$



We can write the Hamiltonian as:

$$\begin{aligned} \hat{H}_{o} &= \hat{1}\hat{H}_{o}\hat{1} \\ &= \sum_{j,k} \left| \mathbf{e}_{j} \right\rangle \left\langle \mathbf{e}_{j} \left| \hat{H}_{o} \right| \mathbf{e}_{k} \right\rangle \left\langle \mathbf{e}_{k} \right| = \sum_{k} \left| \mathbf{E}_{k} \right| \mathbf{e}_{k} \right\rangle \left\langle \mathbf{e}_{k} \right| \end{aligned}$$

$$\sum_{j} |\mathbf{e}_{j}\rangle\langle\mathbf{e}_{j}| = \hat{\mathbf{1}}$$

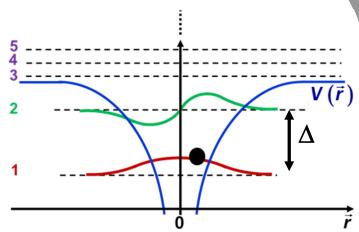
$$\langle\mathbf{e}_{j}|\mathbf{e}_{k}\rangle = \delta_{jk}$$

## Particle in a Potential Well: A Two Level System (TLS)

Assume the Hilbert space is restricted to only the two lowest two energy states of  $\hat{H}_o$ :

$$|\mathbf{e_1}\rangle\langle\mathbf{e_1}|+|\mathbf{e_2}\rangle\langle\mathbf{e_2}|=\mathbf{\hat{1}}$$
  $\longrightarrow$ 

New approximate completeness Two Level System (TLS) approximation



#### The Hamiltonian becomes:

$$\hat{\boldsymbol{H}}_{\boldsymbol{o}} | \mathbf{e}_{\boldsymbol{1}} \rangle = \boldsymbol{E}_{\boldsymbol{1}} | \mathbf{e}_{\boldsymbol{1}} \rangle$$

$$\hat{H}_{o}\left|\mathbf{e_{2}}\right\rangle = E_{2}\left|\mathbf{e_{2}}\right\rangle$$

$$\hat{H}_{o} = \hat{1}\hat{H}_{o}\hat{1}$$

$$= E_{1} |e_{1}\rangle\langle e_{1}| + E_{2} |e_{2}\rangle\langle e_{2}|$$

#### Make the following mapping:

$$|\mathbf{e_1}\rangle \rightarrow \begin{bmatrix} \mathbf{0} \\ \mathbf{1} \end{bmatrix}$$
 and  $|\mathbf{e_2}\rangle \rightarrow \begin{bmatrix} \mathbf{1} \\ \mathbf{0} \end{bmatrix}$ 

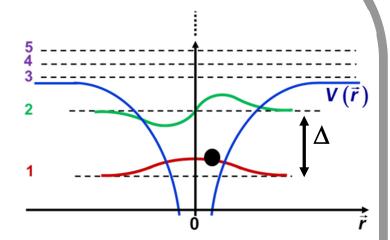
$$\begin{split} \hat{H}_o &= E_1 \Big| e_1 \Big\rangle \Big\langle e_1 \Big| + E_2 \Big| e_2 \Big\rangle \Big\langle e_2 \Big| \\ &= \begin{bmatrix} E_2 & 0 \\ 0 & E_1 \end{bmatrix} \qquad \qquad \Delta = E_2 - E_1 \\ &= \frac{E_1 + E_2}{2} + \begin{bmatrix} \Delta/2 & 0 \\ 0 & -\Delta/2 \end{bmatrix} \\ &= \frac{E_1 + E_2}{2} + \frac{\Delta}{2} \hat{\sigma}_z \end{split}$$

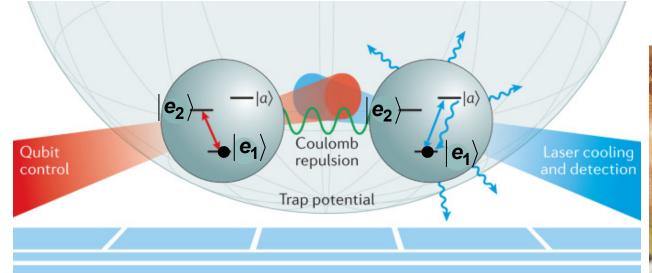
Same as the Hamiltonian of a spin 1/2 in a DC magnetic field !!!

## **A Trapped Ion Qubit**

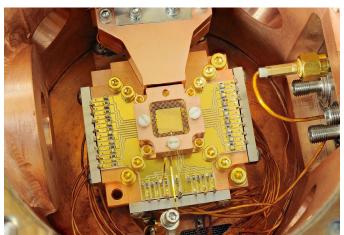
#### Make the following mapping:

$$|e_1\rangle \rightarrow \begin{bmatrix} 0 \\ 1 \end{bmatrix} \rightarrow |1\rangle$$
 and  $|e_2\rangle \rightarrow \begin{bmatrix} 1 \\ 0 \end{bmatrix} \rightarrow |0\rangle$ 
Logical
"1" qubit





Trap electrodes



An ion-trap chip, NIST (2011)

## A Detour on Linear Algebra

Consider the Hamiltonian  $\hat{H}_o$  whose eigenvalues and eigenstates have been found:

$$\hat{H}_{o}\left|\mathbf{e}_{j}\right\rangle = E_{j}\left|\mathbf{e}_{j}\right\rangle$$

$$\sum_{j} |\mathbf{e}_{j}\rangle\langle\mathbf{e}_{j}| = \hat{\mathbf{1}}$$
$$\langle\mathbf{e}_{j}|\mathbf{e}_{k}\rangle = \delta_{jk}$$

Now consider what happens when we add another term to the original Hamiltonian to get a new Hamiltonian:

$$\hat{H} = \hat{H}_o + \hat{O}$$

We can write the new Hamiltonian as:

$$\begin{split} \hat{H} &= \hat{1}\hat{H}_{o}\hat{1} + \hat{1}\hat{O}\hat{1} \\ &= \sum_{j,k} \left| \mathbf{e}_{j} \right\rangle \left\langle \mathbf{e}_{j} \left| \hat{H}_{o} \right| \mathbf{e}_{k} \right\rangle \left\langle \mathbf{e}_{k} \right| + \sum_{j,k} \left| \mathbf{e}_{j} \right\rangle \left\langle \mathbf{e}_{j} \left| \hat{O} \right| \mathbf{e}_{k} \right\rangle \left\langle \mathbf{e}_{k} \right| \\ &= \sum_{k} \left| \mathbf{E}_{k} \right| \mathbf{e}_{k} \right\rangle \left\langle \mathbf{e}_{k} \right| + \sum_{j,k} \left| \mathbf{O}_{jk} \right| \mathbf{e}_{j} \right\rangle \left\langle \mathbf{e}_{k} \right| \end{split}$$

## Particle in a Potential Well Interacting with Light

The classical expression for the potential energy of a charged particle (charge q) in an electromagnetic field is (see Part I):

$$-q\vec{E}(t)\cdot\vec{r}$$
Electric field at the location of the particle

$$\vec{r} = xe_x + ye_y + ze_z$$

$$\vec{E}(t) = \hat{n}E_o \cos(\omega t)$$

$$\vec{E}(t) \cdot \vec{r} = E_o(\hat{n}\cdot\vec{r})\cos(\omega t)$$

 $\hat{n}$  is a unit vector in the direction of the electric field polarization

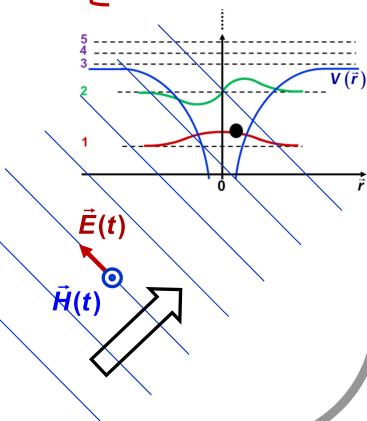
We add this energy to the Hamiltonian of the particle confined in a 1D potential:

$$\hat{H}(t) = \frac{\hat{p}^2}{2m} + V(\hat{r}) - q\vec{E}(t).\hat{r}$$

$$= \frac{\hat{p}^2}{2m} + V(\hat{r}) - qE_o(\hat{n}.\hat{r})\cos(\omega t)$$

$$= \hat{H}_o + \hat{H}_i(t)$$

Hamiltonian becomes time-dependent !!!



**Two Level System (TLS) Approximation** 

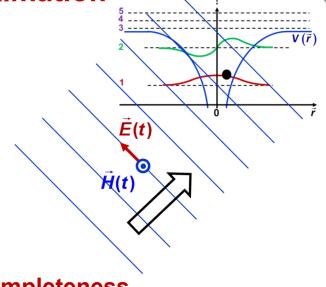
$$\hat{H}(t) = \hat{H}_o + \hat{H}_i(t) = \frac{\hat{p}^2}{2m} + V(\hat{r}) - qE_o(\hat{n}.\hat{r})\cos(\omega t)$$

Assume a Hilbert space consisting of only the two lowest energy states of  $\hat{H}_0$ :

$$\hat{\boldsymbol{H}}_{o}\left|\mathbf{e}_{1}\right\rangle = \boldsymbol{E}_{1}\left|\mathbf{e}_{1}\right\rangle$$

$$\hat{\boldsymbol{H}}_{\mathbf{o}} | \mathbf{e_2} \rangle = \boldsymbol{E_2} | \mathbf{e_2} \rangle$$

$$|e_1\rangle\langle e_1|+|e_2\rangle\langle e_2|=\hat{1}$$
 —— Approximate completeness Two Level System (TLS) approximation



#### Hamiltonian becomes:

$$\begin{split} \hat{H}(t) &= \hat{H}_{o} - qE_{o}\left(\hat{n}.\hat{\vec{r}}\right)\cos(\omega t) \\ &= \hat{1}\hat{H}_{o}\hat{1} - \hat{1}qE_{o}\left(\hat{n}.\hat{\vec{r}}\right)\cos(\omega t)\hat{1} \\ &= E_{1}|\mathbf{e}_{1}\rangle\langle\mathbf{e}_{1}| + E_{2}|\mathbf{e}_{2}\rangle\langle\mathbf{e}_{2}| \\ &- qE_{o}\cos(\omega t) \begin{bmatrix} \langle\mathbf{e}_{1}|\hat{n}.\hat{\vec{r}}|\mathbf{e}_{1}\rangle|\hat{\mathbf{e}}_{1}\rangle\langle\mathbf{e}_{1}| + \langle\mathbf{e}_{2}|\hat{n}.\hat{\vec{r}}|\mathbf{e}_{2}\rangle|\hat{\mathbf{e}}_{2}\rangle\langle\mathbf{e}_{2}| \\ &+ \langle\mathbf{e}_{1}|\hat{n}.\hat{\vec{r}}|\mathbf{e}_{2}\rangle|\mathbf{e}_{1}\rangle\langle\mathbf{e}_{2}| + \langle\mathbf{e}_{2}|\hat{n}.\hat{\vec{r}}|\mathbf{e}_{1}\rangle|\mathbf{e}_{2}\rangle\langle\mathbf{e}_{1}| \end{bmatrix} \end{split}$$

## **Dipole Matrix Elements**

#### Hamiltonian becomes:

$$\hat{H}(t) = E_1 |\mathbf{e}_1\rangle \langle \mathbf{e}_1| + E_2 |\mathbf{e}_2\rangle \langle \mathbf{e}_2|$$

$$-qE_0 \cos(\omega t) \left[ \langle \mathbf{e}_1|\hat{\mathbf{n}}.\hat{\vec{r}}|\mathbf{e}_2\rangle |\mathbf{e}_1\rangle \langle \mathbf{e}_2| + \langle \mathbf{e}_2|\hat{\mathbf{n}}.\hat{\vec{r}}|\mathbf{e}_1\rangle |\mathbf{e}_2\rangle \langle \mathbf{e}_1| \right]$$

#### **Dipole matrix element:**

$$d_{12} = \left\langle \mathbf{e_1} \middle| \hat{n}.\hat{\vec{r}} \middle| \mathbf{e_2} \right\rangle = \int d^3\vec{r} \ \phi_1^* \left( \vec{r} \right) \hat{n}.\vec{r} \phi_2 \left( \vec{r} \right) = \int d^3\vec{r} \ \phi_1^* \left( \vec{r} \right) \left( n_x x + n_y y + n_z z \right) \phi_2 \left( \vec{r} \right)$$

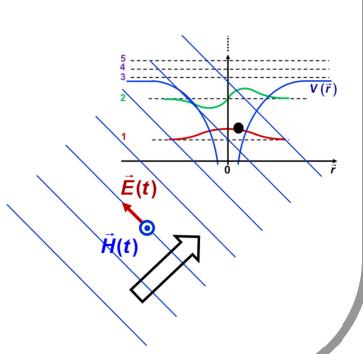
$$d_{21} = d_{12}^* = \langle \mathbf{e_2} | \hat{n}.\hat{\vec{r}} | \mathbf{e_1} \rangle$$

#### **Assume:**

$$d_{12} = d_{21} = d$$

#### **Hamiltonian becomes:**

$$\hat{H}(t) = E_1 |\mathbf{e}_1\rangle \langle \mathbf{e}_1| + E_2 |\mathbf{e}_2\rangle \langle \mathbf{e}_2| - qE_0 d\cos(\omega t) [|\mathbf{e}_1\rangle \langle \mathbf{e}_2| + |\mathbf{e}_2\rangle \langle \mathbf{e}_1|]$$



## **Mapping to a Spin Hamiltonian**

#### Make the following mapping:

$$|\mathbf{e_1}\rangle \rightarrow \begin{bmatrix} \mathbf{0} \\ \mathbf{1} \end{bmatrix}$$
 and  $|\mathbf{e_2}\rangle \rightarrow \begin{bmatrix} \mathbf{1} \\ \mathbf{0} \end{bmatrix}$ 

#### The Hamiltonian becomes:

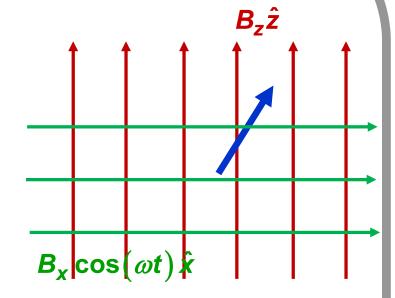
High becomes: 
$$\hat{H}(t) = E_1 | e_1 \rangle \langle e_1 | + E_2 | e_2 \rangle \langle e_2 | \\ -qE_0 d \cos(\omega t) \left[ | e_1 \rangle \langle e_2 | + | e_2 \rangle \langle e_1 | \right] \\ = \begin{bmatrix} E_2 & 0 \\ 0 & E_1 \end{bmatrix} - qE_0 d \cos(\omega t) \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$
 For a 1D potential well 
$$= \frac{E_1 + E_2}{2} + \frac{\Delta}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} - qE_0 d \cos(\omega t) \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$
 
$$= \frac{E_1 + E_2}{2} + \frac{\Delta}{2} \hat{\sigma}_z - qE_0 d \cos(\omega t) \hat{\sigma}_x$$
 Spin Hamiltonian !!!

The Hamiltonian, and therefore the physics, is that of spin 1/2 in a DC z-directed magnetic field and an AC x-directed magnetic field!!!!!

## A Single Spin ½ Qubit in DC and AC Magnetic Fields

#### The Hamiltonian was:

$$\hat{H}(t) = \mu_{B}B_{z}\hat{\sigma}_{z} + \mu_{B}B_{x}\cos(\omega t)\hat{\sigma}_{x}$$
$$= \frac{\Delta}{2}\hat{\sigma}_{z} + \kappa\cos(\omega t)\hat{\sigma}_{x}$$



$$\hat{H}(t) = \frac{\Delta}{2}\hat{\sigma}_{z} - qE_{o}d\cos(\omega t)\hat{\sigma}_{x}$$
$$= \frac{\Delta}{2}\hat{\sigma}_{z} + \kappa\cos(\omega t)\hat{\sigma}_{x}$$

#### **Assume zero detuning:**

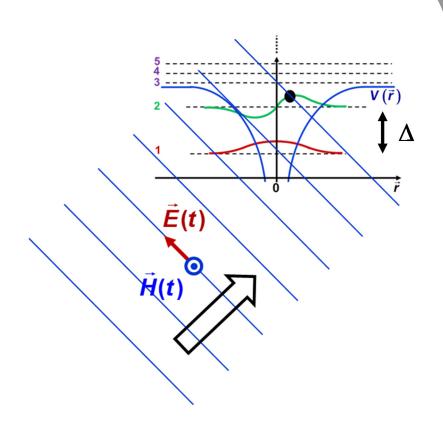
$$\Delta = \boldsymbol{E_2} - \boldsymbol{E_1} = \hbar \boldsymbol{\omega}$$

#### **Need to solve:**

$$i\hbar \frac{\partial \big| \psi(t) \big\rangle}{\partial t} = \hat{H}(t) \big| \psi(t) \big\rangle$$

### Subject to the initial condition:

$$\left|\psi(t=0)\right\rangle = \left|\mathbf{e_2}\right\rangle = \begin{bmatrix}\mathbf{1}\\\mathbf{0}\end{bmatrix}$$



**Need to solve:** 

$$i\hbar \frac{\partial \left|\psi(t)\right\rangle}{\partial t} = \hat{H}(t)\left|\psi(t)\right\rangle$$

Subject to the initial condition:

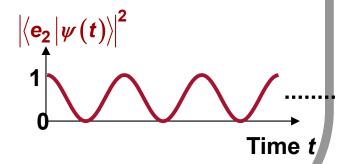
$$|\psi(t=0)\rangle = |\mathbf{e_2}\rangle = \begin{bmatrix} 1\\0 \end{bmatrix}$$

Solution is (from lecture 15, see also the Appendix):

$$\begin{aligned} \left| \psi(t) \right\rangle &= \mathrm{e}^{-i\frac{\omega}{2}t} \cos \left( \frac{\kappa}{2\hbar} t \right) \left| \mathbf{e}_{2} \right\rangle - i \mathrm{e}^{+i\frac{\omega}{2}t} \sin \left( \frac{\kappa}{2\hbar} t \right) \left| \mathbf{e}_{1} \right\rangle \\ &= \mathrm{e}^{-i\frac{\omega}{2}t} \cos \left( \frac{qE_{o}d}{2\hbar} t \right) \left| \mathbf{e}_{2} \right\rangle + i \mathrm{e}^{+i\frac{\omega}{2}t} \sin \left( \frac{qE_{o}d}{2\hbar} t \right) \left| \mathbf{e}_{1} \right\rangle \end{aligned}$$

Probability of finding the electron in the initial upper state at later time *t*:

$$\left|\left\langle \mathbf{e_2} \left| \psi(t) \right\rangle \right|^2 = \cos^2 \left( \frac{qE_od}{2\hbar} t \right) = \frac{1}{2} + \frac{1}{2} \cos \left( \frac{qE_od}{\hbar} t \right)$$



 $\vec{\mathcal{H}}(t)$ 

Probability is oscillating at the frequency:

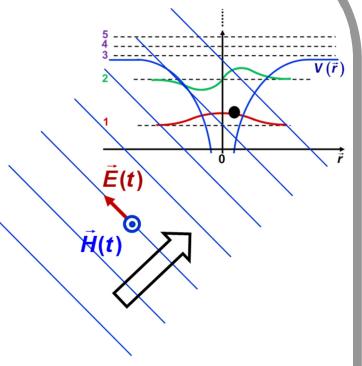
$$\Omega = \frac{|qE_0d|}{\hbar}$$
 Rabi frequency

#### Solution is:

$$\left|\psi(t)\right\rangle = e^{-i\frac{\omega}{2}t}\cos\left(\frac{qE_{o}d}{2\hbar}t\right)\left|e_{2}\right\rangle + ie^{+i\frac{\omega}{2}t}\sin\left(\frac{qE_{o}d}{2\hbar}t\right)\left|e_{1}\right\rangle$$

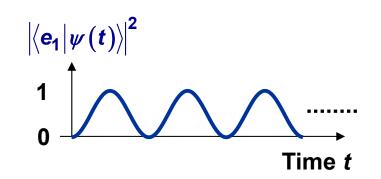
Probability of finding the electron in the lower state at later time *t*:

$$\left|\left\langle \mathbf{e_1} \middle| \psi(t) \right\rangle \right|^2 = \sin^2 \left( \frac{qE_0d}{2\hbar}t \right) = \frac{1}{2} - \frac{1}{2}\cos \left( \frac{qE_0d}{\hbar}t \right)$$



Probability is oscillating at the frequency:

$$\Omega = \frac{|qE_o d|}{\hbar}$$
 Rabi frequency

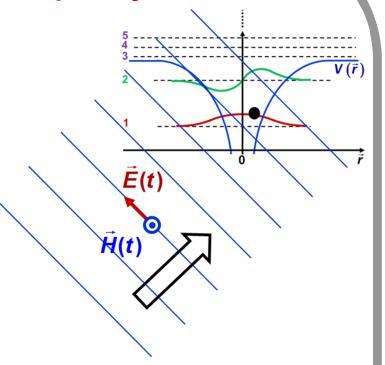


#### **Initial condition:**

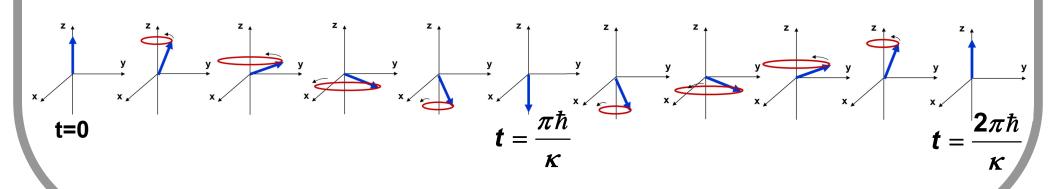
$$\left|\psi\left(t=0\right)\right\rangle = \left|\mathbf{e_2}\right\rangle = \begin{bmatrix}\mathbf{1}\\\mathbf{0}\end{bmatrix}$$

#### Solution is (from lecture 15, see also the Appendix):

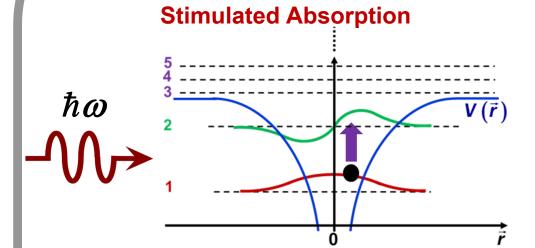
$$\begin{aligned} \left| \psi(t) \right\rangle &= \mathrm{e}^{-i\frac{\omega}{2}t} \cos\left(\frac{\kappa}{2\hbar}t\right) \left| \mathbf{e}_{2} \right\rangle - i \mathrm{e}^{+i\frac{\omega}{2}t} \sin\left(\frac{\kappa}{2\hbar}t\right) \left| \mathbf{e}_{1} \right\rangle \\ &= \mathrm{e}^{-i\frac{\omega}{2}t} \cos\left(\frac{qE_{o}d}{2\hbar}t\right) \left| \mathbf{e}_{2} \right\rangle + i \mathrm{e}^{+i\frac{\omega}{2}t} \sin\left(\frac{qE_{o}d}{2\hbar}t\right) \left| \mathbf{e}_{1} \right\rangle \end{aligned}$$

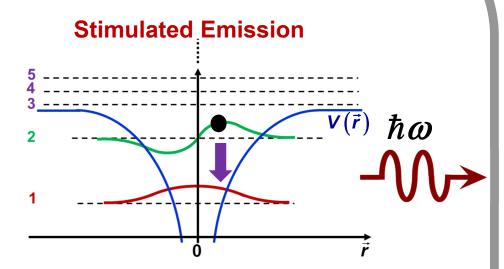


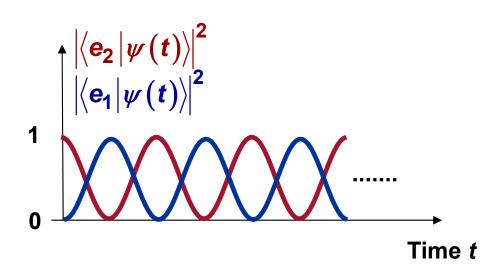
#### If you want to visualize the dynamics of the quantum state:



## **Rabi Oscillations: An Interpretation**

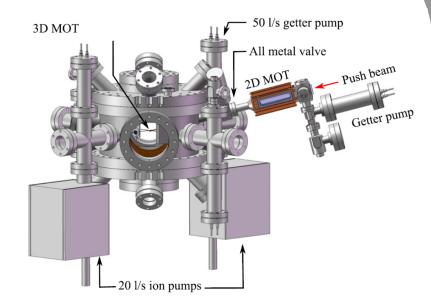




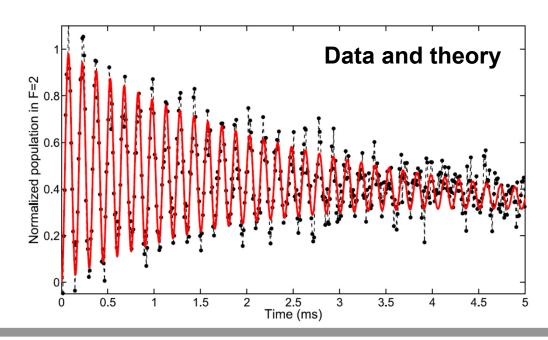


## **Rabi Oscillations in Cold Rubidium Atoms**

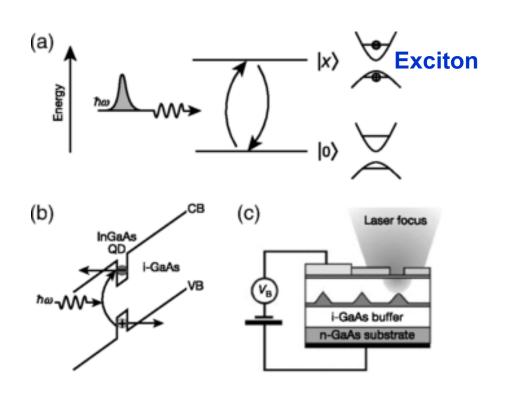
#### **Driven Rabi oscillation in Rubidium atoms**

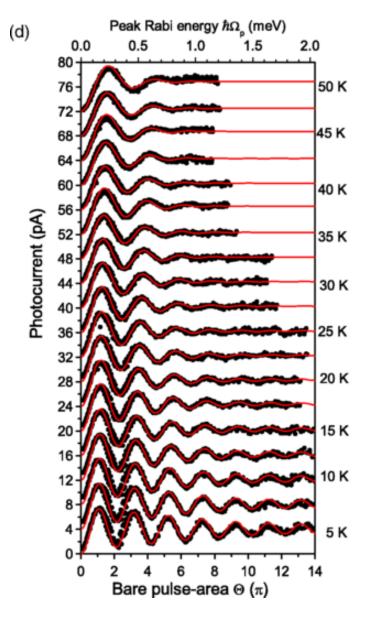


**New Journal of Physics, 13 065021 (2011)** 



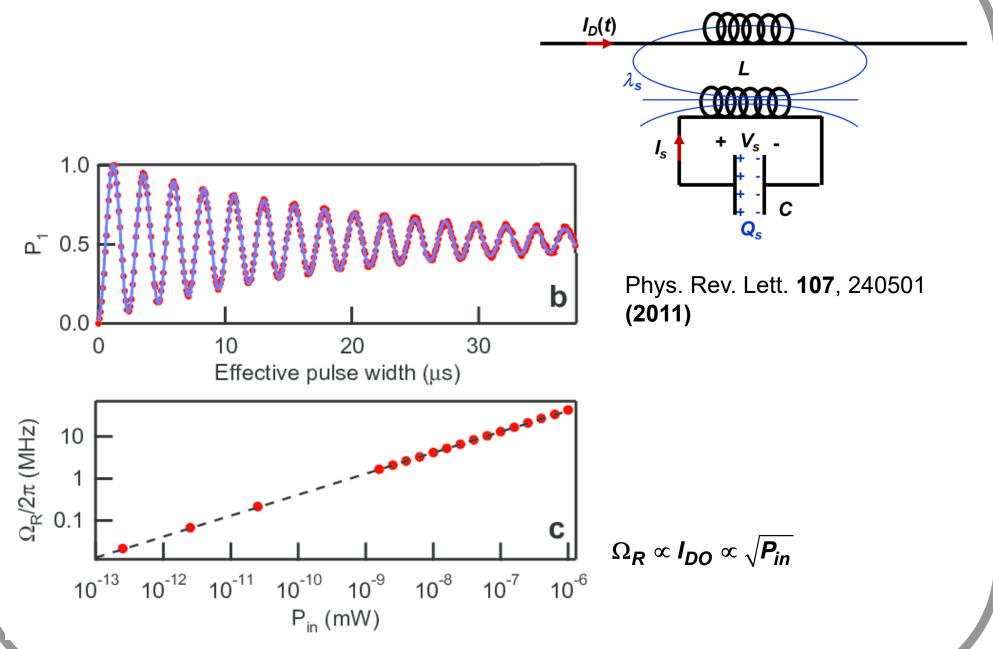
## Rabi Oscillations in Semiconductor Quantum Dots



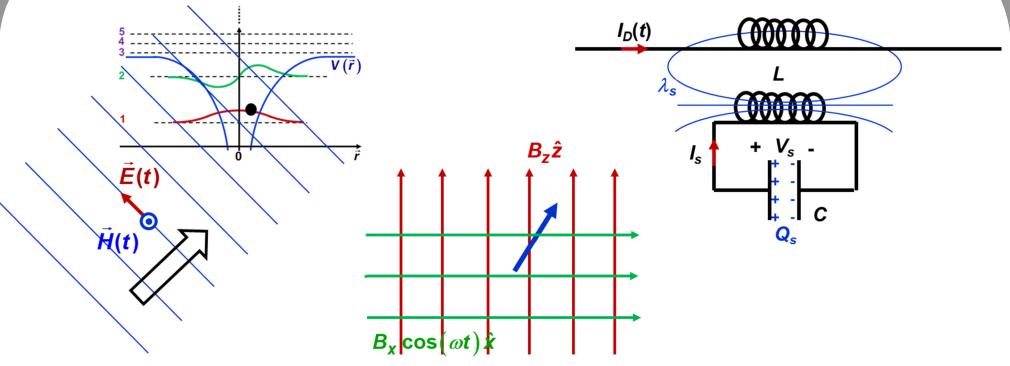


Rev. Mod. Phys., 87, 347 (2015)

## Rabi Oscillations in Superconducting Qubits



## **The Spin Hamiltonians of Two Level Systems**



Note that all these three TLS have a (relevant) Hilbert space of dimension 2 and a Hamiltonian of the same general form:

$$\hat{H}(t) = A + B\hat{\sigma}_z + C\cos(\omega t)\hat{\sigma}_x$$

Suppose we make the following mapping:

$$|\mathbf{e_1}\rangle \rightarrow \begin{bmatrix} \mathbf{0} \\ \mathbf{1} \end{bmatrix}$$
 and  $|\mathbf{e_2}\rangle \rightarrow \begin{bmatrix} \mathbf{1} \\ \mathbf{0} \end{bmatrix}$ 

And suppose under this mapping:

$$\hat{H}(t) = \frac{\Delta}{2}\hat{\sigma}_z + \kappa \cos(\omega t)\hat{\sigma}_x$$

**Need to solve:** 

$$i\hbar \frac{\partial \big|\psi(t)\big\rangle}{\partial t} = \hat{H}(t)\big|\psi(t)\big\rangle$$

With the initial condition:

$$|\psi(t=0)\rangle = \alpha |\mathbf{e_1}\rangle + \beta |\mathbf{e_2}\rangle = \begin{bmatrix} \beta \\ \alpha \end{bmatrix}$$

**Need to solve:** 

$$i\hbar \frac{\partial \left|\psi(t)\right\rangle}{\partial t} = \hat{H}(t)\left|\psi(t)\right\rangle$$

**Assume:** 

$$\left|\psi(t)\right\rangle = a(t) e^{i\frac{\Delta}{2\hbar}t} \left| e_1 \right\rangle + b(t) e^{-i\frac{\Delta}{2\hbar}t} \left| e_2 \right\rangle = \left| b(t) e^{-i\frac{\Delta}{2\hbar}t} \right| a(t) e^{+i\frac{\Delta}{2\hbar}t}$$

LHS:

$$i\hbar \frac{\partial |\psi(t)\rangle}{\partial t} = i\hbar \frac{\partial}{\partial t} \begin{bmatrix} b(t)e^{-i\frac{\Delta}{2\hbar}t} \\ a(t)e^{i\frac{\Delta}{2\hbar}t} \end{bmatrix} = \begin{bmatrix} e^{-i\frac{\Delta}{2\hbar}t}i\hbar \frac{\partial b(t)}{\partial t} \\ e^{i\frac{\Delta}{2\hbar}t}i\hbar \frac{\partial a(t)}{\partial t} \end{bmatrix} + \frac{\Delta}{2}\hat{\sigma}_z \begin{bmatrix} b(t)e^{-i\frac{\Delta}{2\hbar}t} \\ a(t)e^{i\frac{\Delta}{2\hbar}t} \end{bmatrix}$$

RHS:

$$\hat{H}(t)|\psi(t)\rangle = \frac{\Delta}{2}\hat{\sigma}_{z}\begin{bmatrix}b(t)e^{-i\frac{\Delta}{2\hbar}t}\\a(t)e^{i\frac{\Delta}{2\hbar}t}\end{bmatrix} + \kappa\cos(\omega t)\begin{bmatrix}a(t)e^{i\frac{\Delta}{2\hbar}t}\\b(t)e^{-i\frac{\Delta}{2\hbar}t}\end{bmatrix}$$

$$i\hbar \frac{\partial \left| \psi(t) \right\rangle}{\partial t} = \hat{H}(t) \left| \psi(t) \right\rangle$$

$$\Rightarrow \begin{bmatrix} e^{-i\frac{\Delta}{2\hbar}t} i\hbar \frac{\partial b(t)}{\partial t} \\ e^{i\frac{\Delta}{2\hbar}t} i\hbar \frac{\partial a(t)}{\partial t} \end{bmatrix} = \kappa \cos(\omega t) \begin{bmatrix} a(t) e^{i\frac{\Delta}{2\hbar}t} \\ b(t) e^{-i\frac{\Delta}{2\hbar}t} \end{bmatrix}$$

$$\Rightarrow i\hbar \frac{\partial}{\partial t} \begin{bmatrix} b(t) \\ a(t) \end{bmatrix} = \kappa \begin{vmatrix} a(t)e^{i\frac{\Delta}{\hbar}t}\cos(\omega t) \\ b(t)e^{-i\frac{\Delta}{\hbar}t}\cos(\omega t) \end{vmatrix}$$

Assume zero detuning:  $\Delta = \hbar \omega$  and using the rotating wave approximation:

$$i\hbar \frac{\partial}{\partial t} \begin{bmatrix} b(t) \\ a(t) \end{bmatrix} = \frac{\kappa}{2} \begin{bmatrix} a(t) \\ b(t) \end{bmatrix} \xrightarrow{\text{Solution}} \begin{bmatrix} b(t) \\ a(t) \end{bmatrix} = \begin{bmatrix} A \\ C \end{bmatrix} \cos\left(\frac{\kappa}{2\hbar}t\right) + \begin{bmatrix} B \\ D \end{bmatrix} \sin\left(\frac{\kappa}{2\hbar}t\right)$$

$$i\hbar \frac{\partial}{\partial t} \begin{bmatrix} b(t) \\ a(t) \end{bmatrix} = \frac{\kappa}{2} \begin{bmatrix} a(t) \\ b(t) \end{bmatrix} \xrightarrow{\text{Solution}} \begin{bmatrix} b(t) \\ a(t) \end{bmatrix} = \begin{bmatrix} A \\ C \end{bmatrix} \cos\left(\frac{\kappa}{2\hbar}t\right) + \begin{bmatrix} B \\ D \end{bmatrix} \sin\left(\frac{\kappa}{2\hbar}t\right)$$

#### **Initial conditions:**

$$\begin{bmatrix} b(t) \\ a(t) \end{bmatrix}_{t=0} = \begin{bmatrix} \beta \\ \alpha \end{bmatrix}$$

$$i\hbar \frac{\partial}{\partial t} \begin{bmatrix} b(t) \\ a(t) \end{bmatrix}_{t=0} = \frac{\kappa}{2} \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

#### **Final solution:**

$$\begin{bmatrix} b(t) \\ a(t) \end{bmatrix} = \begin{bmatrix} \beta \\ \alpha \end{bmatrix} \cos\left(\frac{\kappa}{2\hbar}t\right) - i \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \sin\left(\frac{\kappa}{2\hbar}t\right)$$

$$\Rightarrow \left| \psi(t) \right\rangle = \begin{bmatrix} b(t) e^{-i\frac{\Delta}{2\hbar}t} \\ a(t) e^{+i\frac{\Delta}{2\hbar}t} \end{bmatrix} = \begin{bmatrix} \beta e^{-i\frac{\Delta}{2\hbar}t} \\ \alpha e^{+i\frac{\Delta}{2\hbar}t} \end{bmatrix} \cos\left(\frac{\kappa}{2\hbar}t\right) - i \begin{bmatrix} \alpha e^{-i\frac{\Delta}{2\hbar}t} \\ \beta e^{+i\frac{\Delta}{2\hbar}t} \end{bmatrix} \sin\left(\frac{\kappa}{2\hbar}t\right)$$