QO2 - Lecture 5

Until now, I have stated that the interaction Hamiltonian is given by: $H_I = -\vec{d}\cdot\vec{E}$

dipole moment ↗ ↖ electric field

where does this come from?

We can start from (see QO1 notes):

$$\hat{H} = \frac{1}{2m}\left(\hat{p} - qA(\hat{r},t)\right)^2 + qU(\hat{r},t)$$

Is this a unique Hamiltonian? No! We can choose a function $F(r,t)$, called the guage, and some new potentials defined by:

$$A'(r,t) = A(r,t) + \nabla F(r,t)$$
$$U'(r,t) = U(r,t) - \frac{\partial}{\partial t}F(r,t)$$

Then the <u>observable</u> electric and magnetic fields given by:

$$B(r,t) = \nabla \times A(r,t)$$
$$E(r,t) = -\frac{\partial}{\partial t}A(r,t) - \nabla U(r,t)$$

are completely unchanged!

The Coulomb Guage

We choose a guage such that $\nabla\cdot A(r,t) = 0$.

eg. recall a plane EM wave:

$$\vec{E} = \vec{E}_0\cos(\omega t - k\cdot r)$$
$$\vec{B} = \frac{\vec{k}\times\vec{E}_0}{\omega}\cos(\omega t - k\cdot r)$$
$$\vec{E}_0\cdot\vec{k} = 0$$

Then it is easy to verify

$$A_\perp = -\frac{E_0}{\omega}\sin(\omega t - k\cdot r)$$

$$U = 0$$

Satisfy the equations for E & B.

Thus $$E(r,t) = -\frac{\partial}{\partial t}A_\perp(r,t)$$

Then our Hamiltonian, for this choice of guage, becomes:

$$H = \frac{1}{2m}(p - qA_\perp)^2 + V_{coul}$$

only contains field variables

only contains atomic variables

Advantage: Clear separation of field & atomic variables.

Now, recall $\hat{p} = -i\hbar\nabla$.

$$\vec{\nabla}\cdot(\vec{A}_\perp\psi) = \vec{A}_\perp\cdot(\vec{\nabla}\psi) + \underbrace{(\vec{\nabla}\cdot\vec{A}_\perp)}_{0}\psi$$

$$= \vec{A}_\perp\cdot\vec{\nabla}\psi$$

Thus $$\vec{\nabla}\cdot\vec{A}_\perp\psi - \vec{A}_\perp\cdot\vec{\nabla}\psi = 0 = [\vec{\nabla},\vec{A}_\perp]$$

and $$[\vec{p},\vec{A}_\perp] = 0$$

So the Hamiltonian becomes:

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

$$\hat{H}_0 = \frac{p^2}{2m} + \hat{V}_{coul}$$

$$\hat{H}_I = -\frac{q}{m}\hat{p}\cdot\hat{A}_\perp(r,t) + \frac{q^2A_\perp^2(r,t)}{2m}$$

The Göppert-Mayer Guage

We're not done yet! We now apply the guage transform:

$$F(r,t) = -(\vec{r}-\vec{r}_0)\cdot A_\perp(r_0,t)$$

where $\vec{r}_0$ is the location of the nucleus. This looks like we're moving to the reference frame of the atom!

Then applying this we have:

$$A'(\hat{r},t) = A_\perp(\hat{r},t) - A_\perp(r_0,t)$$

$$U'(\hat{r},t) = U_{coul}(r) + (\hat{r}-r_0)\cdot\frac{d}{dt}A_\perp(r_0,t)$$

Recall that $E(r,t) = -\frac{d}{dt}A_\perp(r,t)$

and calling $\hat{D} = q(\hat{r}-r_0)$

we have:

$$H = \frac{1}{2m}(\hat{p} - qA'(\hat{r},t))^2 + \hat{V}_{coul}(r,t) - \hat{D}\cdot\hat{E}(r_0,t)$$

Long Wavelength Approximation (or: Dipole Approximation)

Assume the vector potential is constant over the extent of the atom.

$$\lambda \gtrsim 100\,nm$$

$$a_0 \sim 0.1\ nm$$

So this looks like a good approximation.

So we replace $\vec{A}'(\hat{r},t)$ with $A'(r_0,t) = 0$.

And finally

$$\boxed{H = H_0 + H_I \qquad H_0 = \frac{p^2}{2m} + V_{coul}(\hat{r}),\quad H_I = -\hat{D}\cdot E(r_0,t)}$$

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A Two Level Atom Coupled to an EM Field

Recall we studied interactions of the type:

$$\hat{H}_1(t) = \hat{W}\cos(\omega t + \phi)$$

Here, this amounts to a sinusoidal E-field:

$$\vec{E}(\vec{r}_0, t) = \vec{E}(\vec{r}_0)\cos(\omega t + \phi)$$

with the identification $\hat{W} = -\hat{\vec{D}} \cdot \vec{E}(\vec{r}_0)$

We found that transitions were only significant when

$E_k = E_i \pm \hbar\omega$, within $\Delta\omega = \pi/T$, where T is the duration of the interaction.

We found that $P_{i\to k} = \frac{T\,|W_{ki}|^2}{4}\left(\frac{2\pi}{\hbar}\right)\delta_T(E_k - E_i - \hbar\omega)$

Then set $\hbar\Omega_R \equiv W_{ki} = -\langle k|\hat{\vec{D}}\cdot\vec{\varepsilon}\,|i\rangle E(\vec{r}_0)$ where $\vec{E}(\vec{r}_0) = \vec{\varepsilon}\,E(\vec{r}_0)$

$$= -d\,E(\vec{r}_0)$$

where Ω_R is the Rabi frequency and d is the dipole moment in the direction $\vec{\varepsilon}$ of the electric field.

Then $P_{i\to k} = \frac{T\,\Omega_R^2\hbar}{4}\,2\pi\,\delta_T(E_k - E_i - \hbar\omega)$

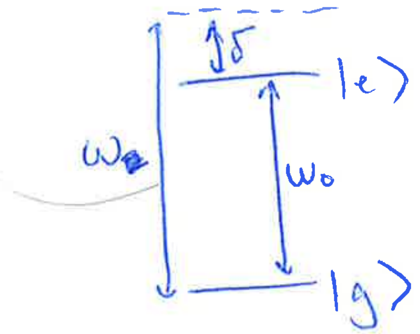
Define the DETUNING $\delta = \omega - |E_i - E_k|/\hbar$, the laser frequency shift above or below resonance.

Then $\delta_T(\hbar\delta) = \frac{2\hbar\sin^2(\delta T/2)}{\pi T(\delta\hbar)^2} = \frac{T}{2\pi\hbar}\,\frac{\sin^2(\delta T/2)}{(\delta T/2)^2}$

$$\boxed{P_{i\to k} = \frac{\Omega_R^2 T^2}{4}\left(\frac{\sin(\delta T/2)}{(\delta T/2)}\right)^2}\ \ast\!\ast$$

How does this compare to an exact solution?

Rabi Oscillation between 2 levels



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

It is convenient to define $H_0|g\rangle = -\frac{\hbar\omega_0}{2}|g\rangle$

$$H_0|e\rangle = \frac{\hbar\omega_0}{2}|e\rangle$$

In the basis of the two states,

$$H_0 = \begin{pmatrix} \frac{\hbar\omega_0}{2} & 0 \\ 0 & \hbar\omega_0/2 \end{pmatrix}$$

What about $\hat{H}_I$? Recall the $\langle i|H_I|i\rangle = 0$, so

$$H_I = \begin{pmatrix} 0 & \hbar\Omega_R \\ \hbar\Omega_R & 0 \end{pmatrix}\cos(\omega t + \phi)$$

Remembering the Pauli matrices:

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

we see that:

$$\hat{H} = \frac{\hbar\omega_0}{2}\sigma_z + \hbar\Omega_R\sigma_x\cos(\omega t + \phi)$$

This is difficult to solve exactly, since its time dependent.

We have some other tricks!

The rotating frame

To solve this problem, we move into a frame of reference that rotates about the z-axis @ frequency ω_F:

$$|\psi'\rangle = R_z^\dagger(\omega_F t)|\psi\rangle \quad , \quad R_z^\dagger(\theta) = e^{i\theta\sigma_z/2}$$

How does the Schrödinger equation change?

$$\hat{H}|\psi\rangle = i\hbar\frac{d}{dt}|\psi\rangle \quad , \quad \text{substitute } |\psi\rangle = R_z(\omega_F t)|\psi'\rangle$$

$$\frac{d}{dt}|\psi\rangle = \left(\frac{d}{dt}R_z(\omega_F t)\right)|\psi'\rangle + R_z(\omega_F t)\frac{d}{dt}|\psi'\rangle$$

and
$$\frac{d}{dt}R_z(\omega_F t) = \frac{-i\omega_F\sigma_z}{2}R_z(\omega_F t)$$

Now multiply on the left by $R^\dagger(\cdot)$ and the SE becomes:

$$R_z^\dagger(\omega_F t)\hat{H}R_z(\omega_F t)|\psi'\rangle = \frac{\hbar\omega_F\sigma_z}{2}|\psi'\rangle + i\hbar\frac{d}{dt}|\psi'\rangle$$

Then we have:

$$\underbrace{\left[R_z^\dagger(\omega_F t)\hat{H}R_z(\omega_F t) - \frac{\hbar\omega_F}{2}\sigma_z\right]}_{H'}|\psi'\rangle = i\hbar\frac{d}{dt}|\psi'\rangle$$

So moving into the rotating frame consists of:

$$\boxed{\begin{aligned} &\hat{H} \rightarrow \hat{H}' = R_z^\dagger(\omega_F t + \phi_F)\hat{H}(t)R_z(\omega_F t + \phi_F) - \frac{\hbar\omega_F}{2}\sigma_z \\ \text{and} \quad &|\psi\rangle \rightarrow R_z^\dagger|\psi'\rangle \end{aligned}}$$

Recall that for Pauli matrices:

$$e^{i\theta(\hat{n}\cdot\vec{\sigma})} = \mathbb{I}\cos\theta + i(n\cdot\hat{\sigma})\sin\theta$$

Then $R_z(\omega_F t + \phi_F) = \begin{pmatrix} e^{i(\omega_F t+\phi_F)/2} & 0 \\ 0 & e^{-i(\omega_F t+\phi_F)/2} \end{pmatrix}$

and then:

$$R_z^{+}\sigma_x R_z = \begin{pmatrix} 0 & e^{-i(\omega_F t+\phi_F)} \\ e^{i(\omega_F t+\phi_F)} & 0 \end{pmatrix}$$

Now remember

$$\hat{H}' = \frac{\hbar(\omega_0-\omega_F)}{2}\sigma_z + \hbar\Omega_R R_z^{+}\sigma_x R_z\cos(\omega t)$$

(Note: $R_z^{+}\sigma_z R_z = \sigma_z$)

and that $\cos(\omega t) = \dfrac{e^{i\omega t}+e^{-i\omega t}}{2}$

then the second term is:

$$\frac{\hbar\Omega_R}{2}\begin{pmatrix} 0 & e^{-i\phi_F/2}\left[e^{-i(\omega_F+\omega)t}+e^{-i(\omega_F-\omega)t}\right] \\ e^{i\phi_F/2}\left[e^{i(\omega_F+\omega)t}+e^{i(\omega_F-\omega)t}\right] & 0 \end{pmatrix}$$

There are two rotating terms, one @ $\omega_F+\omega$ (FAST) and one at $\omega_F-\omega$ (SLOW). THE ROTATING WAVE APPROXIMATION ignores the fast-rotating terms, so the second term becomes:

$$= \frac{\hbar \Omega_R}{2} \begin{pmatrix} 0 & e^{-i\phi_F/2} e^{-i(\omega_F - \omega)t} \\ e^{i\phi_F/2} e^{i(\omega_F - \omega)t} & 0 \end{pmatrix}$$

Now we choose $\omega_F = \omega$ and:

$$= \frac{\hbar}{2} \begin{pmatrix} 0 & \Omega_R \\ \Omega_R & 0 \end{pmatrix}$$

where I have redefined Ω_R as a complex number with amplitude $\hbar|\Omega_R| = -dE(\vec{r}_0)$ and phase ϕ_F.

Then finally, we have:

$$H' = \frac{\hbar}{2}\left(-\delta \sigma_z + \Omega_R \sigma_x\right)$$

$$\boxed{H' = \frac{\hbar}{2} \begin{pmatrix} -\delta & \Omega_R \\ \Omega_R & +\delta \end{pmatrix}} \quad *\ *\ *$$

This Hamiltonian is time-independant! (and easily solveable).

In fact, we already solved it!

- Rabi oscillations @ $\Omega = \sqrt{\delta^2 + \Omega_R^2}$
- Amplitude of oscillations $= \frac{\Omega_R^2}{\delta^2 + \Omega_R^2}$