Atom-Light Interaction: 2-Level Approximation

Comparison to the Classical Lorentz atom

Goal: To understand why the Lorentz model works so well, and to determine its limits of validity

Classical Equation of Motion:

$$\boxed{\left(\frac{d^2}{dt^2}+\omega_0^2\right)\vec{r}=\frac{e}{m}\vec{E}}$$

will derive similar equation for $\langle\hat{\vec{r}}\rangle$

Equation of Motion for $\langle\hat{\vec{r}}\rangle$. First step:

$$\langle\hat{\vec{r}}\rangle=\langle\psi|\hat{\vec{r}}|\psi\rangle=(a_1^*,a_2^*)\begin{pmatrix}0 & \vec{r}_{12}\\ \vec{r}_{21} & 0\end{pmatrix}\begin{pmatrix}a_1\\ a_2\end{pmatrix}$$

$$=a_1^*a_2\,\vec{r}_{12}+a_2^*a_1\,\vec{r}_{21}=\vec{r}_{12}\left(a_1^*a_2+a_2^*a_1\right)$$

(choose phase to make $\vec{r}_{12}$ real)

We need an expression for $\frac{d^2}{dt^2}\langle\vec{r}\rangle$

We can find it from the S. E., i. e., the eqs for the *a*'s back when we first set up the Rabi problem.

We pick linear polarization so $\vec{\varepsilon}E_0$ is real-valued and $V_{12}=V_{21}=V$. In that case the eqs for the *a*'s are

$$\hbar\dot{a}_1^*=i\left(E_1a_1^*+Va_2^*\right)$$
$$\hbar\dot{a}_2=-i\left(E_2a_2+Va_1\right)$$

With this we have

$$\frac{d}{dt}a_1^*a_2=\left(\dot{a}_1^*a_2+a_1^*\dot{a}_2\right)$$
$$=-i\underbrace{\frac{E_2-E_1}{\hbar}}_{\omega_0}a_1^*a_2-i\frac{V}{\hbar}\left(|a_1|^2-|a_2|^2\right)$$

Differentiating again gives us

$$\frac{d^2}{dt^2}\left(a_1^*a_2\right)=-\omega_0^2\,a_1^*a_2-\frac{\omega_0V}{\hbar}\left(|a_1|^2-|a_2|^2\right)$$
$$-i\hbar\frac{d}{dt}\left[\frac{V}{\hbar}\left(|a_1|^2-|a_2|^2\right)\right]$$

Looking at the eq. for $\langle\hat{\vec{r}}\rangle$ suggests we should add the complex conjugate and multiply w/ $\vec{r}_{12}$

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We pick linear polarization so $\vec{\mathcal{E}}E_0$ is real-valued and $V_{12} = V_{21} = V$. In that case the eqs for the *a*'s are

$$\hbar \dot{a}_1^* = i(E_1 a_1^* + V a_2^*)$$

$$\hbar \dot{a}_2 = -i(E_2 a_2 + V a_1)$$

With this we have

$$\frac{d}{dt} a_1^* a_2 = (\dot{a}_1^* a_2 + a_1^* \dot{a}_2)$$

$$= -i \underbrace{\frac{E_2 - E_1}{\hbar}}_{\omega_0} a_1^* a_2 - i \frac{V}{\hbar}(|a_1|^2 - |a_2|^2)$$

Differentiating again gives us

$$\frac{d^2}{dt^2}(a_1^* a_2) = -\omega_0^2 a_1^* a_2 - \frac{\omega_0 V}{\hbar}(|a_1|^2 - |a_2|^2)$$

$$-i\hbar \frac{d}{dt}\left[\frac{V}{\hbar}(|a_1|^2 - |a_2|^2)\right]$$

Looking at the eq. for $\langle \hat{\vec{r}} \rangle$ suggests we should add the complex conjugate and multiply w/ $\vec{r}_{12}$

This gives us

$$\left(\frac{d^2}{dt^2} + \omega_0^2\right)\langle \hat{\vec{r}} \rangle = \frac{2\omega_0 \vec{r}_{12} V}{\hbar}(|a_1|^2 - |a_2|^2)$$

$$= \frac{2\omega_0}{\hbar} \vec{r}_{12} (\vec{r}_{12} \cdot \vec{E}) (|a_1|^2 - |a_2|^2)$$

$\vec{r}_{12} = \langle 1 | \hat{\vec{r}} | 2 \rangle$: dipole matrix element

To wrap up, we need to know a bit about real, multilevel atoms. (We will revisit this soon)

Pick linear polarization so $\vec{\mathcal{E}}$ is real-valued.
Pick quantization axis along $\vec{\mathcal{E}}$ $\Rightarrow$ $\vec{r}_{12} = r_{12} \vec{\mathcal{E}}$

$$\boxed{\left(\frac{d^2}{dt^2} + \omega_0^2\right)\langle \hat{r} \rangle = \frac{2\omega_0 r_{12}^2}{\hbar} \vec{E} (|a_1|^2 - |a_2|^2)}$$

Atom-Light Interaction: 2-Level Approximation

This gives us

$$\left(\frac{d^2}{dt^2}+\omega_0^2\right)\langle\hat{\vec{\wp}}\rangle = \frac{2\omega_0\vec{\wp}_{12}V}{\hbar}\left(|a_1|^2-|a_2|^2\right)$$

$$= \frac{2\omega_0}{\hbar}\vec{\wp}_{12}\left(\vec{\wp}_{12}\cdot\vec{E}\right)\left(|a_1|^2-|a_2|^2\right)$$

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Pick linear polarization so $\vec{\mathcal{E}}$ is real-valued.
Pick quantization axis along $\vec{\mathcal{E}}$ ⇨ $\vec{\wp}_{12} = \wp_{12}\vec{\mathcal{E}}$

$$\boxed{\left(\frac{d^2}{dt^2}+\omega_0^2\right)\langle\hat{\vec{\wp}}\rangle = \frac{2\omega_0\wp_{12}^2}{\hbar}\vec{E}\left(|a_1|^2-|a_2|^2\right)}$$

Compare to Classical Equation of Motion

$$\boxed{\left(\frac{d^2}{dt^2}+\omega_0^2\right)\vec{\wp} = \frac{e}{m}\vec{E}}$$

The two eqs. have the same form if $|a_1|^2\sim 1$, $|a_2|^2\sim 0$

This is the case for $\Delta \gg \chi$

Or when $\chi \ll \Gamma$

Limit of weak Excitation !

↑ Decay rate of $|2\rangle$

Oscillator Strength $\boxed{f = \frac{2m\omega_0}{\hbar e}\wp_{12}^2}$

$$\boxed{\left(\frac{d^2}{dt^2}+\omega_0^2\right)\langle\hat{\vec{\wp}}\rangle = \frac{e}{m}f\vec{E}}$$

Exactly like the classical equation, but with modified polarizability !

End 02-04-2022

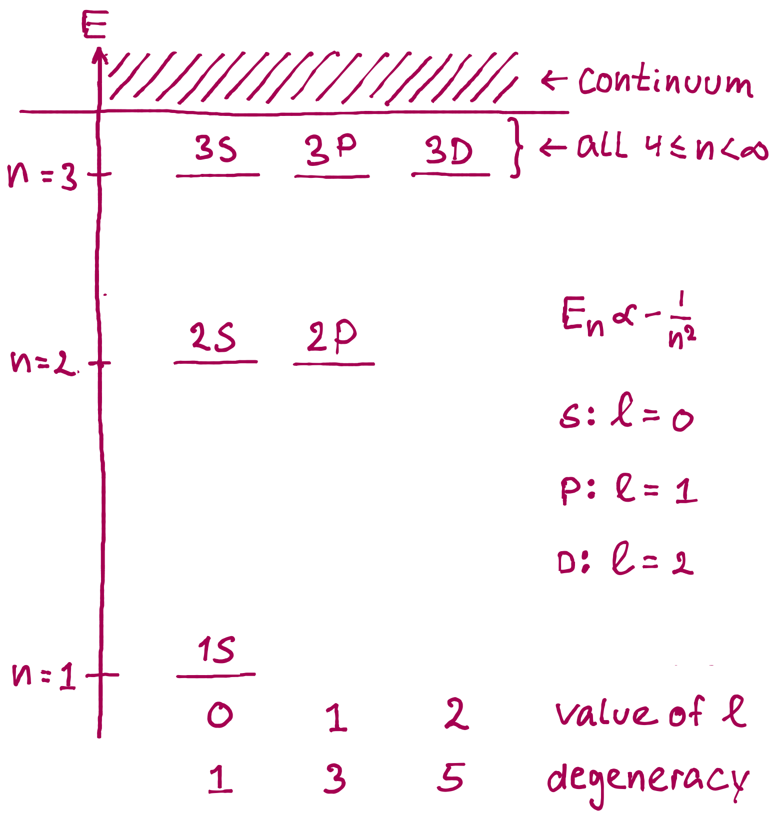
Atom-Light Interaction: Multi-Level Atoms

Starting point – the Hydrogen atom

$$H_a = \frac{p^2}{2m} - \frac{1}{4\pi\varepsilon_0}\frac{e^2}{|\vec{r}|}$$

$$V_{ext}(\vec{r},\vec{R},t) = -e\vec{r}\cdot\vec{E}(\vec{R},t)$$

$\vec{r}$: relative $\quad\vec{R}$: center-of-mass



Note: Frequencies for transitions $n\to n'$, $n''\to n'''$ are very different ⇨ near-resonant approx. with a single transition frequency $\omega\sim\omega_0$

Levels $|n\ell\rangle$ are generally degenerate with respect to the quantum number m, so we cannot isolate a 2-level system only through its transition frequency.

We must therefore consider Selection Rules

Interaction matrix element

$$\langle n'\ell'n'|V_{ext}|n\ell m\rangle \propto \int_{-\infty}^{\infty} dr^3\, \varphi^*_{n'\ell'm'}(\vec{r})\,\vec{r}\,\varphi_{n\ell m}(\vec{r})$$

Wavefunction parity is even/odd depending on ℓ

$$\varphi_{n\ell m}(\vec{r}) = (-1)^{\ell}\varphi_{n\ell m}(-\vec{r})$$

⇨ $\langle|V|\rangle$ can be non-zero only if $(\ell-\ell')$ is odd.

This is the Parity Selection Rule !

Atom-Light Interaction: Multi-Level Atoms

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Next: We will find selection rules that derive from the angular symmetry of the matrix element

We need to develop the proper math language

➡ spherical basis vectors and harmonics

Consider an arbitrary set of orthonormal basis vectors $\vec{\varepsilon}_i, \vec{\varepsilon}_j, \vec{\varepsilon}_k$. We can always write

$$\vec{r} = (\vec{r}\cdot\vec{\varepsilon}_i)\vec{\varepsilon}_i + (\vec{r}\cdot\vec{\varepsilon}_j)\vec{\varepsilon}_j + (\vec{r}\cdot\vec{\varepsilon}_k)\vec{\varepsilon}_k$$

Cartesian basis: $\vec{\varepsilon}_i = \vec{\varepsilon}_x \quad \vec{\varepsilon}_j = \vec{\varepsilon}_y \quad \vec{\varepsilon}_k = \vec{\varepsilon}_z$

(real-valued)

Spherical basis:

(complex-valued)

$$\begin{cases} \vec{\varepsilon}_i = \vec{\varepsilon}_1 = -\frac{1}{\sqrt{2}}(\vec{\varepsilon}_x + i\vec{\varepsilon}_y) \\ \vec{\varepsilon}_j = \vec{\varepsilon}_{-1} = \frac{1}{\sqrt{2}}(\vec{\varepsilon}_x - i\vec{\varepsilon}_y) \\ \vec{\varepsilon}_h = \vec{\varepsilon}_0 = \vec{\varepsilon}_z \end{cases}$$

Reminder: Scalar products of complex vectors

Dirac notation	Regular notation
$\{\lvert a\rangle + i\lvert b\rangle, \lvert c\rangle\}$	$(\vec{a}+i\vec{b})\cdot\vec{c}$
$= (\langle a\rvert - i\langle b\rvert)\lvert c\rangle$	$= \vec{a}\cdot\vec{c} - i\,\vec{b}\cdot\vec{c}$
$= \langle a\vert c\rangle - i\langle b\vert c\rangle$	(anti-linear in 1st factor)

Atom-Light Interaction: Multi-Level Atoms

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Scalar Products in the spherical basis

Homework: prove the relations

$$\boxed{\vec{\varepsilon}_q^{\,*} = (-1)^q\vec{\varepsilon}_q, \qquad \vec{\varepsilon}_{q'}\cdot\vec{\varepsilon}_q = \delta_{qq'}, \qquad \vec{\varepsilon}_{q'}\cdot\vec{\varepsilon}_q^{\,*} = (-1)^q\delta_{-q'q}}$$

Next: Rewrite $\vec{r}\cdot\vec{\varepsilon}_q$ in polar coordinates

$$\vec{r}\cdot\vec{\varepsilon}_x = x = r\sin\theta\cos\varphi$$

$$\vec{r}\cdot\vec{\varepsilon}_y = y = r\sin\theta\sin\varphi$$

$$\vec{r}\cdot\vec{\varepsilon}_z = z = r\cos\theta$$

Compare to the Spherical Harmonics

$$Y_1^0(\theta,\varphi) = \sqrt{\frac{3}{4\pi}}\cos\theta, \quad Y_1^{\pm1}(\theta,\varphi) = \pm\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{\pm i\varphi}$$

$$\left.\begin{aligned} x &= -r\sqrt{\frac{2\pi}{3}}(Y_1^1 - Y_1^{-1}) \\ y &= ir\sqrt{\frac{2\pi}{3}}(Y_1^1 + Y_1^{-1}) \\ z &= r\sqrt{\frac{4\pi}{3}}Y_1^0 \end{aligned}\right\} \Rightarrow \boxed{\vec{r}\cdot\vec{\varepsilon}_q = r\sqrt{\frac{4\pi}{3}}\,Y_1^q}$$

Atom-Light Interaction: Multi-Level Atoms

Scalar Products in the spherical basis

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This finally gives us $\vec{\varepsilon}_q$ in the spherical basis:

$$\boxed{\vec{r}=\sum_{q=0,\pm1}(\vec{r}\cdot\vec{\varepsilon}_q)\vec{\varepsilon}_q = r\sqrt{\frac{4\pi}{3}}\sum_{q=0,\pm1}Y_1^q\vec{\varepsilon}_q}$$

End Lecture 02-04-2022 **End math preamble**

Back to the Matrix Elements

First:

$$V_{ext}=-e\vec{r}\cdot\vec{E}(t)$$

electric dipole interaction

$$\vec{E}(t)=\frac{1}{2}E_0\left(\vec{\varepsilon}_q e^{-i\omega t}+\vec{\varepsilon}_q^{\,*}e^{i\omega t}\right)$$

$$=\frac{1}{2}E_0\left(\vec{\varepsilon}_q e^{-i\omega t}+(-1)^q\vec{\varepsilon}_q e^{i\omega t}\right)$$

electric field polarization $\vec{\varepsilon}_q$

$$V_{ext}=-\sqrt{\pi/3}\,eE_0r\Big(\sum_{q'}Y_1^{q'}\overbrace{\underbrace{\vec{\varepsilon}_{q'}\Big)\cdot\Big(\vec{\varepsilon}_q}_{\delta_{q'q}}e^{-i\omega t}+(-1)^q\vec{\varepsilon}_{-q}e^{i\omega t}}^{\delta_{q'(-q)}}\Big)$$

$$\boxed{V_{ext}\propto r\left(Y_1^q e^{-i\omega t}+(-1)^q Y_1^{-q}e^{i\omega t}\right)}$$

Atom-Light Interaction: Multi-Level Atoms

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electric dipole interaction

$$\vec{E}(t) = \frac{1}{2}E_0\left(\vec{\varepsilon}_q e^{-i\omega t} + \vec{\varepsilon}_q^{\,*} e^{i\omega t}\right)$$

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$$V_{ext} = -\sqrt{\pi/3}\, eE_0 r \left(\sum_{q'} Y_1^{q'} \underbrace{\overbrace{\vec{\varepsilon}_{q'}\Big)\cdot\Big(\vec{\varepsilon}_q}_{\delta_{q'q}} e^{-i\omega t} + (-1)^q \vec{\varepsilon}_{-q}}^{\delta_{q'(-q)}} e^{i\omega t}\right)$$

$$\boxed{V_{ext} \propto r\left(Y_1^q e^{-i\omega t} + (-1)^q Y_1^{-q} e^{i\omega t}\right)}$$

The matrix element = overlap integral of the form

$$V_{21} = \langle n'\ell'm' | V_{ext} | n\ell m\rangle$$

$$\propto \int_{\mathbb{R}^3} d^3r\, \varphi^*_{n'\ell'm'}(\vec{r}) \overbrace{r\left(Y_1^q e^{-i\omega t} + (-1)^q Y_1^{-q} e^{i\omega t}\right)}^{V_{ext}} \varphi_{n\ell m}(\vec{r})$$

where the wavefunctions $\varphi_{n\ell m}(\vec{r}) = R_{n\ell}(r)\, Y_\ell^m(\theta,\varphi)$

$$V_{21} = \langle n'\ell'm' | V_{ext} | n\ell m\rangle$$

$$= \mathcal{R} \times \underbrace{\int_{4\pi} d\Omega \left(Y_{\ell'}^{m'}\right)^* \left(Y_1^q e^{-i\omega t} + (-1)^q Y_1^{-q} e^{i\omega t}\right) Y_\ell^m}_{\text{angular integral}}$$

radial integral

Thus, to within a constant factor

$$V_{21} = \langle \ell'm' |\, Y_1^q e^{-i\omega t} + (-1)^q Y_1^{-q} e^{i\omega t} \,| \ell m\rangle = V_{12}^*$$

From the RWA, we know the resonant terms are

Atom-Light Interaction: Multi-Level Atoms

$$\boxed{\begin{aligned} i\dot{a}_1 &= -\tfrac{1}{2}\left(\chi_{12}e^{-i\omega t} + \chi_{21}^{*}e^{i\omega t}\right)a_2 \\ i\dot{a}_2 &= \omega_{21}a_2 - \tfrac{1}{2}\left(\chi_{21}e^{-i\omega t} + \chi_{12}^{*}e^{i\omega t}\right)a_1 \end{aligned}}$$

$$\boxed{\begin{aligned} ic_1(t) &= -\tfrac{1}{2}\left(\chi_{12}e^{-i2\omega t} + \chi_{21}^{*}\right)c_2(t) \\ i\dot{c}_2(t) &= (\omega_{21}-\omega)c_2(t) - \tfrac{1}{2}\left(\chi_{21} + \chi_{12}^{*}e^{i2\omega t}\right)c_1(t) \end{aligned}}$$

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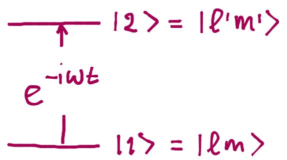

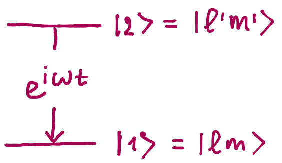

Atom-Light Interaction: Multi-Level Atoms

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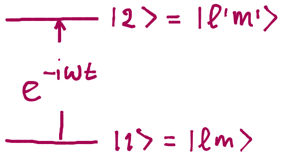

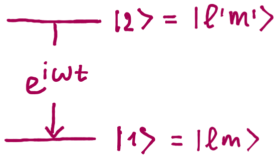

And thus in the RWA we get (use $(Y_\ell^m)^* = (-1)^m Y_\ell^{-m}$)

$$\boxed{\begin{aligned} V_{21} &\propto \langle \ell'm' | Y_1^q e^{-i\omega t} | \ell m\rangle \\ V_{12} &\propto \langle \ell m | (-1)^q Y_1^{-q} e^{i\omega t} | \ell'm'\rangle \end{aligned}}$$

dropping the factor $(-1)^q$

$$\boxed{\begin{aligned} V_{21} &\propto \int d\Omega\, (Y_{\ell'}^{m'})^* Y_1^q Y_\ell^m \propto \langle 1,q;\ell m | \ell'm'\rangle \\ V_{12} &\propto \int d\Omega\, (Y_\ell^m)^* Y_1^{-q} Y_{\ell'}^{m'} \propto \langle 1,-q;\ell'm' | \ell m\rangle \end{aligned}}$$

Clebsch-Gordan coefficients

Next: We can understand this as conservation of angular momentum when a photon is absorbed or emitted

Selection Rules for Electric Dipole Transitions

Atom-Light Interaction: Multi-Level Atoms

Reminder: Addition of Angular Momenta

Let $\vec{J} = \vec{J}_1 + \vec{J}_2$ ⇨ **eigenstates** $\left\{ \begin{array}{l} |j_1 m_1\rangle \\ |j_2 m_2\rangle \\ |j m\rangle \end{array} \right.$

We can write $|jm\rangle$ **in the basis** $|j_1 m_1\rangle |j_2 m_2\rangle$

$$|jm\rangle = \overbrace{\sum_{m_1, m_2} |j_1 m_1; j_2 m_2\rangle\langle j_1 m_1; j_2 m_2|}^{\text{identity}} jm\rangle$$

$$= \sum_{m_1 m_2} \underset{\uparrow}{\langle j_1 m_1; j_2 m_2 | jm\rangle} |j_1 m_1; j_2 m_2\rangle$$

Clebsch-Gordan coefficients

CG's are non-zero when

Conservation of
Angular Momentum

$$\boxed{\begin{array}{c} |j_1 - j_2| \leq j \leq j_1 + j_2 \\ m_1 + m_2 = m \end{array}}$$

Going back to the matrix element $V_{21} \neq 0$

when $|1q\rangle$ **combined w/** $|\ell m\rangle$ **is consistent w/** $|\ell' m'\rangle$

↑ "photon" AM ↑ ground state AM ↑ excited state AM

The corresponding Selection Rules are

$$\ell' - \ell = 0, \pm 1, \quad m' - m = q, \quad q = 0, \pm 1$$

Combining with the Parity Rule, this gives us the

Electric Dipole Selection Rules

$$\boxed{\ell' - \ell = \pm 1, \quad m' - m = q, \quad q = 0, \pm 1}$$