Begin
01-30-2023

Atom-Light Interaction: 2-Level Approximation

Comparison to the Classical Lorentz atom

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

Classical Equation of Motion:

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

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

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

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

$$=a_1^*a_2\,\vec{r}_{12}+a_2^*a_1\,\vec{r}_{21}=\vec{r}_{12}\,(a_1^*a_2+a_1a_2^*)$$

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

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

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 $\vec{\mathcal{E}}E_0$ is real-valued and $V_{12}=V_{21}=V$ ➡ **The eqs for the *a* 's are**

$$\hbar\dot{a}_1^*=i(E_1a_1^*+Va_2^*)$$

$$\hbar\dot{a}_2=-i(E_2a_2+Va_1)$$

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

$$\frac{d^2}{dt^2}(a_1^*a_2)=-\omega_0^2\,a_1^*a_2-\frac{\omega_0V}{\hbar}(|a_1|^2-|a_2|^2)$$

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

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

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

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

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 $\langle \hat{\vec{p}} \rangle$ suggests we should add the complex conjugate and multiply w $\vec{p}_{12}$

This gives us

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

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

$\vec{p}_{12} = \langle 1 | \hat{\vec{p}} | 2 \rangle$: 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 $\vec{\mathcal{E}}$ ➡ $\vec{p}_{12} = p_{12}\vec{\mathcal{E}}$

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

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

Compare to Classical Equation of Motion

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

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 !**

Γ: Decay rate of $|2\rangle$

Oscillator Strength

$$f = \frac{2m\omega_0}{\hbar e}p_{12}^2$$

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

Like the classical equation, but with modified polarizability !

Atom-Light Interaction: Multi-Level Atoms

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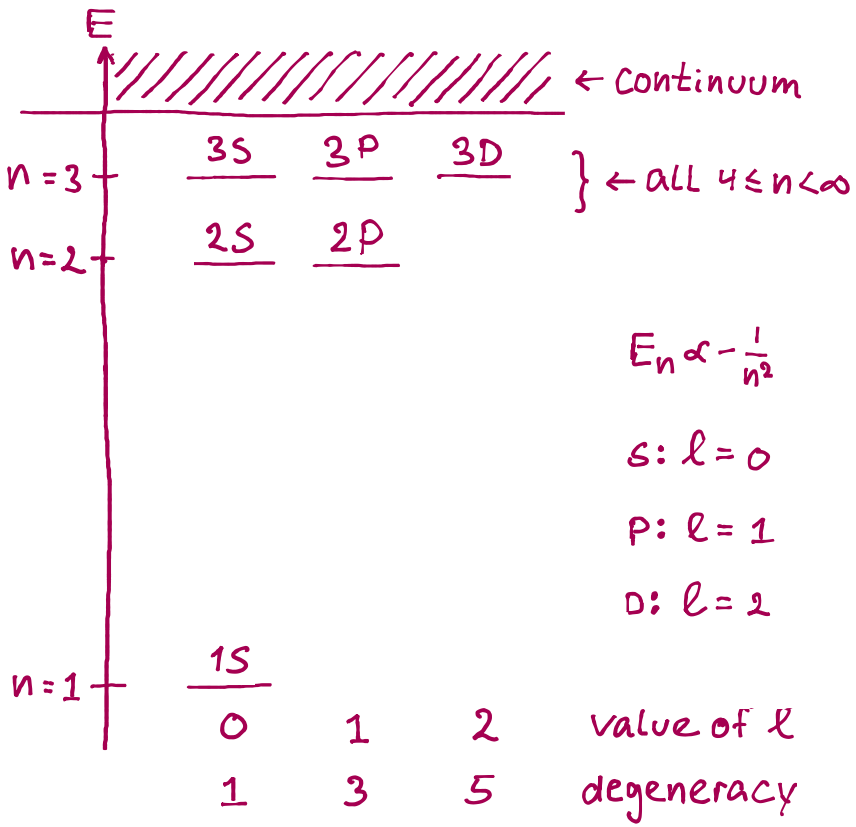
Starting point – the Hydrogen atom

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

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

$\vec{r}$: relative $\vec{R}$: 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

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

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: (real-valued) $\quad \vec{\varepsilon}_i = \vec{\varepsilon}_x,\ \vec{\varepsilon}_j = \vec{\varepsilon}_y,\ \vec{\varepsilon}_k = \vec{\varepsilon}_z$

Spherical basis: (complex-valued)

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

Reminder: Scalar products of complex vectors

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

Atom-Light Interaction: Multi-Level Atoms

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Dirac notation

$$\{|a\rangle + i|b\rangle, |c\rangle\} = (\langle a| - i\langle b|)|c\rangle = \langle a|c\rangle - i\langle b|c\rangle$$

Regular notation

$$(\vec{a} + i\vec{b})\cdot\vec{c} = \vec{a}\cdot\vec{c} - i\vec{b}\cdot\vec{c}$$

(anti-linear in 1st factor)

Math Preamble: The Spherical Basis

(1) Prove the relations (Homework)

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

(2) Show that

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

where

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

$$Y_1^0(\theta,\varphi) = \sqrt{\frac{3}{4\pi}}\cos\theta$$

(Spherical Harmonics)

Atom-Light Interaction: Multi-Level Atoms

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(Spherical Harmonics)

Example:

$$\vec{\varepsilon}_1 = -\frac{1}{\sqrt{2}}(\vec{\varepsilon}_x + i\vec{\varepsilon}_y) \Rightarrow \vec{r}\cdot\vec{\varepsilon}_1 = -\frac{1}{\sqrt{2}}(\vec{r}\cdot\vec{\varepsilon}_x + i\vec{r}\cdot\vec{\varepsilon}_y)$$

Substitute: **(Spherical Coordinates)**

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

$$\vec{r}\cdot\vec{\varepsilon}_1 = r\frac{1}{\sqrt{2}}(\sin\theta\cos\varphi + i\sin\theta\sin\varphi)$$

$$= r\frac{1}{\sqrt{2}}\sin\theta\, e^{i\varphi} = r\sqrt{\frac{4\pi}{3}}\, Y_1^1(\theta,\varphi)$$

Relations for q = 0, -1 follow similarly.

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End Math Preamble

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

End Math Preamble

Back to the Dipole Matrix Elements. First:

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

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

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

electric field polarization

$$V_{ext} = -\sqrt{\pi/3}\, e E_0 r\left(\sum_{q'} Y_1^{q'}\underbrace{\vec{\varepsilon}_{q'}\cdot\vec{\varepsilon}_q}_{\delta_{q'q}}\right)\cdot\overbrace{\left(\vec{\varepsilon}_q e^{-i\omega t} + (-1)^q\vec{\varepsilon}_{-q} e^{i\omega t}\right)}^{\delta_{q'(-q)}}$$

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

Atom-Light Interaction: Multi-Level Atoms

Back to the Matrix Elements. First:

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

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

↑ electric field polarization

$$V_{ext} = -\sqrt{\pi/3}\, e E_0 r \left(\sum_{q'} Y_1^{q'} \underbrace{\vec{\varepsilon}_{q'}}_{\delta_{q'(-q)}}\right)\cdot\left(\vec{\varepsilon}_q e^{-i\omega t} + (-1)^q \vec{\varepsilon}_{-q} e^{i\omega t}\right)$$

$$\delta_{q'q}$$

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

The matrix element = overlap integral

$$\vec{\varepsilon}_1 = -\frac{1}{\sqrt{2}}\left(\vec{\varepsilon}_x + i\vec{\varepsilon}_y\right) \Rightarrow \vec{r}\cdot\vec{\varepsilon}_1 = -\frac{1}{\sqrt{2}}\left(\vec{r}\cdot\vec{\varepsilon}_x + i\vec{r}\cdot\vec{\varepsilon}_y\right)$$

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

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

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

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

↑ radial integral

angular integral

Thus, to within a constant factor

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

Atom-Light Interaction: Multi-Level Atoms

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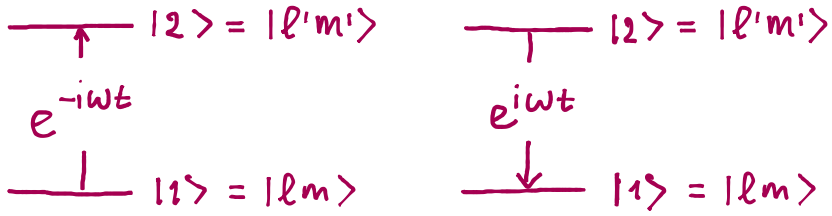
Resonant terms:



Recall from 2-level system:

$$i\dot{a}_1 = -\frac{1}{2}\left(\chi_{12} e^{-i\omega t} + \chi_{21}^* e^{i\omega t}\right) a_2$$

$$i\dot{a}_2 = \omega_{21} a_2 - \frac{1}{2}\left(\chi_{21} e^{-i\omega t} + \chi_{12}^* e^{i\omega t}\right) a_1$$

$$i\dot{C}_1(t) = -\frac{1}{2}\left(\chi_{12} e^{-i2\omega t} + \chi_{21}^*\right) C_2(t)$$

$$i\dot{C}_2(t) = (\omega_{21} - \omega) C_2(t) - \frac{1}{2}\left(\chi_{21} + \chi_{12}^* e^{i2\omega t}\right) C_1(t)$$

(RWA)

$$i\dot{C}_1(t) = -\frac{1}{2}\chi_{21}^* C_2(t)$$

$$i\dot{C}_2(t) = \Delta C_2(t) - \frac{1}{2}\chi_{21} C_1(t)$$

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

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