

# FOMO 2024

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Today, we will be taking the "semiclassical" approach, i.e., treating the atom quantum mechanically while still taking the light to be classical

This means that we get to dig out the Schrödinger equation, and now we can start talking about fun things like coherences + superpositions.

So, let's start w/ the time-dependent Schrödinger equation (TDSE)

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle = \hat{H} |\Psi(t)\rangle$$

— here, we will generally give operators like  $\hat{H}$  (our Hamiltonian) hats

if  $\hat{H}$  is time-independent, this is easy to solve

$$|\Psi(t)\rangle = e^{-i\hat{H}t/\hbar} |\Psi(0)\rangle$$

note: exponentials of operators are not trivial! treat them carefully! (especially in numerics)

How do we then treat the atom-light interaction semiclassically?

The game now is figuring out the Hamiltonian that describes our dynamics accurately.

Let's stick to our beloved two-level atom:



The strongest type of transition that we can drive is the so-called electric dipole transition that arises from the electric dipole of the light + the electric dipole of the atom → call this  $d$

There exist other possible transitions → magnetic dipole, electric quadrupole, etc, all with their own selection rules (which we won't talk about here because our atoms only have 2 levels). That said, our electric dipole is stronger by quite a few orders of magnitude.

We also need an expression for the bare Hamiltonian for the atom when it's unperturbed by the light.

This can take the basic form

$$\hat{H}_0 = \left[ \frac{\hat{p}^2}{2m} + \hat{V}(r) \right]$$

kinetic energy potential binds our single electron to our two-level atom

Note that our two-level atom has one electron: more levels + more electrons lead to more complex behaviour

Thus, with our simple atom, we can sweep complexities under the rug + write

$$\hat{H}_0 = \hbar\omega_0 |e\rangle\langle e|$$

$\hat{H}_0 |e\rangle = \hbar\omega_0 |e\rangle$  ✓  
 $\hat{H}_0 |g\rangle = 0 |g\rangle$  ✓

Why does our electric dipole take the form that it does? (see, e.g., Sec. 4.1 in Gerry + Knight)

One can perform a long, reasonably rigorous derivation using the scalar ( $\phi$ ) and vector ( $\vec{A}$ ) fields of the (classical) light field, as well as Lagrangian/Hamiltonian mechanics, but a more straightforward argument is to make the (very good) electric dipole approximation:

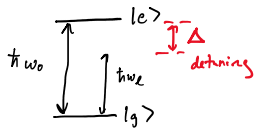
Electric dipole approximation: the  $\vec{E}$  field does not appreciably vary (spatially) over atomic length scales

Optical wavelengths: 400-700 nm } this approximation is solid  
 Atomic scales: 1 Å = 0.1 nm

Then, the  $\vec{E}$  field is roughly constant across our atom, and our solitary electron sees a force  $\vec{F} = -e\vec{E}$

Noting that  $\vec{F} = -\nabla U$ , this gives  $U = +e\vec{r} \cdot \vec{E} = -\vec{d} \cdot \vec{E}$  where  $\vec{d} = -e\vec{r}$  and our full Hamiltonian is  
 ↑ this should be satisfying given what we know about classical electrodynamics  
 $\hat{H} = \hat{H}_0 - \vec{d} \cdot \vec{E}$  where  $\vec{E}$  is fully classical!

Now let's give  $\vec{E}$  the familiar form:  
 $\vec{E}(t) = \hat{e} E_0 \cos(\omega_0 t)$   
 polarization (arrow) field frequency (lower) detuning (arrow)



Let's take a closer look @ the dipole moment: spatial wavefunctions (require knowledge of V(r̄))

Consider  $\langle e | \vec{d} \cdot \vec{E} | e \rangle \propto \langle e | \vec{d} | e \rangle = -e \int d\vec{r} \psi_e^*(\vec{r}) \vec{r} \psi_e(\vec{r})$

This is just a clever way of writing zero! Why?

Quantum spatial eigenstates must have a well-defined parity, i.e.,  $\psi_e(-\vec{r}) = \pm \psi_e(\vec{r})$  (same for  $\psi_g$ )  
 Therefore  $\psi_e^* \psi_e$  has positive parity (again, same for  $\psi_g$ )

∴  $\langle e | \vec{d} | e \rangle = \langle g | \vec{d} | g \rangle = 0$  and  $\vec{d}$  is off-diagonal in the  $\{|e\rangle, |g\rangle\}$  basis.

Thus, because otherwise things are very boring,  $|e\rangle + |g\rangle$  must have opposite parity so that  $\langle e | \vec{d} | g \rangle \neq 0$  selection rules!

$\hat{d}$  as an operator can be written  $\hat{d} = d_{eg} \hat{\sigma}^+ + d_{eg}^* \hat{\sigma}$   $\hat{\sigma} = |g\rangle\langle e|$   
 Taking the dipole moment to be real gives

$\hat{H} = \hbar\omega_0 \hat{\sigma}^+ \hat{\sigma} + \hbar\Omega \cos(\omega_0 t) (\hat{\sigma} + \hat{\sigma}^+)$

$\hat{\sigma}^+ \hat{\sigma} = |e\rangle\langle g|g\rangle\langle e| = |e\rangle\langle e|$   $\Omega = \frac{\vec{E} \cdot d_{eg} E_0}{\hbar}$

This is solid, but time-dependent Hamiltonians are annoying, so let's move into a rotating frame rotating at a frequency  $\omega_0$

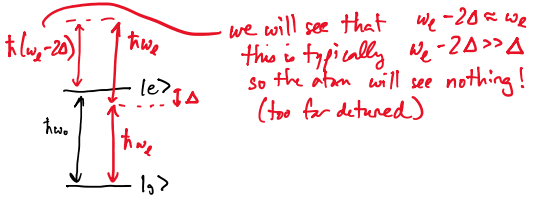
We can do this via a unitary transformation, giving us a set of rotating states  $|\psi_R(t)\rangle = \hat{U}_R(t) |\psi(t)\rangle$

and a rotating Hamiltonian  $\hat{H}_R(t) = \hat{U}_R(t) \hat{H} \hat{U}_R^\dagger(t) + i\hbar \partial_t \hat{U}_R(t) \hat{U}_R^\dagger(t)$

If we take  $\hat{U}_R(t) = \exp(i\omega_0 |e\rangle\langle e| t)$ , then

$\hat{H}_R(t) = \hbar(\omega_0 - \omega_0) \hat{\sigma}^+ \hat{\sigma} + \hbar\Omega \cos(\omega_0 t) [\hat{\sigma} e^{-i\omega_0 t} + \hat{\sigma}^+ e^{i\omega_0 t}]$   
 $= \hbar\Delta \hat{\sigma}^+ \hat{\sigma} + \frac{\hbar\Omega}{2} (\hat{\sigma} (e^{-2i\omega_0 t} + 1) + \hat{\sigma}^+ (e^{2i\omega_0 t} + 1))$

This is exact! However,  $2\omega_0$  is usually very fast ( $2\pi \times 100$  THz), so the atom won't be able to respond



As such, we make the common rotating-wave approximation, which means that we neglect the terms rotating at  $\exp(\pm 2i\omega_0 t) \rightarrow$  they average to zero.

This isn't always a great approximation, but for now it'll do nicely.

$$\hat{H}_R(t) \approx \hat{H}_{RWA} = \hbar \Delta \hat{\sigma}^+ \hat{\sigma} + \frac{\hbar \Omega}{2} (\hat{\sigma} + \hat{\sigma}^+)$$

This is the Hamiltonian for a semi-classical atom-light interaction without dissipation

In our  $\{|e\rangle, |g\rangle\}$  basis, this is a qubit with Hamiltonian

$$\hat{H}_{RWA} = \hbar \begin{pmatrix} \Delta & \Omega/2 \\ \Omega/2 & 0 \end{pmatrix}$$