Chap 1 Early Atomic Physics

This chapter we will go through some basic concepts and get rough sizes that are important for different atomic processes.

Atomic Units Natural units for atoms

Charge $e = 1.602 \times 10^{-19}\,C$

Mass $m_e = 9.109 \times 10^{-31}\,kg$

Ang. mom. $\hbar = 1.055 \times 10^{-34}\,kg\,m^2/s$

Length $a_0 = \hbar^2 / [\frac{e^2}{4\pi\varepsilon_0} m_e] = 0.5292 \times 10^{-10}\,m$

Speed $v_0 = \hbar/(m_e a_0) = 2.188 \times 10^6\,m/s$

Time $t_0 = a_0/v_0 = 24.19 \times 10^{-18}\,s$

Energy $E_0 = e^2/4\pi\varepsilon_0 a_0 = 4.360 \times 10^{-18}\,J = 27.211\,eV$ $\left(= \frac{\hbar^2}{m_e a_0^2}\right)$

Elec. Dip. Mom $p_0 = e a_0 = 8.478 \times 10^{-30}\,Cm$ $(1\text{ Debye} = 3.336 \times 10^{-30}\,Cm = 0.39\,p_0)$

Mag. Dip Mom $\mu_0 = \frac{e}{t_0} a_0^2 = 1.855 \times 10^{-23}\,J/T = 2\mu_B$

Fine structure constant $\alpha = \frac{v_0}{c} = \frac{1}{137.04}$

Bohr H atom - Electron moves in a circle around proton with $m_e v r = n\hbar$ Gives quantized energies, radii, speeds, ...

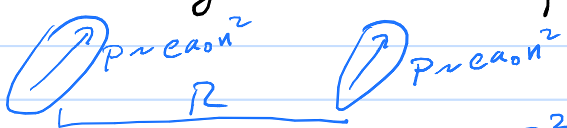
$E_n = -\frac{1}{2} E_0 / n^2$ Note bunching of energy levels at high n

$r_n = a_0 n^2$ Note the increasing size at high n

$v_n = v_0 / n$ Note the slower speed at high n

Typical atoms have almost no interaction at distances larger than few nm. Highly excited atoms have noticeable interaction

Proposal to entangle atomic states using highly excited atoms through electric dipole-dipole interaction.



In terms of frequency $E/h \sim \frac{p^2}{4\pi\varepsilon_0 R^3} = \frac{E_0}{h}\left(\frac{a_0}{R}\right)^3 n^4 \simeq 1\,kHz \frac{n^4}{(R/\mu m)^3}$

$R = 3\,\mu m$, $n = 50$ $E/h \sim 200\,MHz$

More complicated because not permanent dipole moment

You can manipulate highly excited states with microwaves

$\Delta E/h = \frac{E_0}{h}\left(\frac{1}{50^2} - \frac{1}{51^2}\right) = 102\,GHz$

The energies can be shifted with small E-fields

$F \sim \frac{E_0}{a_0 e} \frac{1}{n^4} \sim 5.14\times10^{11}\,V/m\,\frac{1}{n^4} = 5.14\times10^{9}\,V/cm\,/n^4$

At $n = 100$ $F \sim 51\,V/cm$ ~destroys atom

If there is a higher charge $E_n \propto Z^2/n^2$, $r_n \propto n^2/Z$, $v_n \propto \frac{Z}{n}$

X-Rays!

If the electron → muon $r \propto n^2 \frac{m_e}{m_\mu}$, $v \propto \frac{1}{n}$, $E_n \propto \frac{1}{n^2}\frac{m_\mu}{m_e}$

muon catalyzed fusion, exotic atoms

For a charge interacting with electric and magnetic fields, the Hamiltonian is

$$H = \frac{(\vec{p} - q\vec{A})^2}{2m} + q\varphi \qquad \text{where} \quad \vec{E} = -\vec{\nabla}\varphi - \frac{\partial \vec{A}}{\partial t} \qquad \vec{B} = \vec{\nabla} \times \vec{A}$$

Show that Hamilton's equations give the correct equations of motion

$$\dot{x} = \frac{\partial H}{\partial p_x} = \frac{p_x - qA_x}{m} \implies p_x = m\dot{x} + qA_x = mv_x + qA_x(x,y,z,t)$$

$$\dot{p}_x = -\frac{\partial H}{\partial x} = -q\frac{\partial \varphi}{\partial x} + \frac{q}{m}\left[\frac{\partial A_x}{\partial x}(p_x - qA_x) + \frac{\partial A_y}{\partial x}(p_y - qA_y) + \frac{\partial A_z}{\partial x}(p_z - qA_z)\right]$$

$$= -q\frac{\partial \varphi}{\partial x} + q\left(\frac{\partial A_x}{\partial x}v_x + \frac{\partial A_y}{\partial x}v_y + \frac{\partial A_z}{\partial x}v_z\right)$$

$$= m\dot{v}_x + q\frac{\partial A_x}{\partial t} + q v_x\frac{\partial A_x}{\partial x} + q v_y\frac{\partial A_x}{\partial y} + q v_z\frac{\partial A_x}{\partial z}$$

Shuffle

$$m\dot{v}_x = -q\left(\frac{\partial \varphi}{\partial x} + \frac{\partial A_x}{\partial t}\right) + q v_y\left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right) - q v_z\left(\frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x}\right)$$

$$= q\left[E_x + v_y B_z - v_z B_y\right] \checkmark$$

To understand the implications, let's look at two examples

1) a hydrogen atom in a constant, uniform B-field
2) a hydrogen atom in a plane light wave

Example 1) $\varphi(\vec{r}) = \frac{e}{4\pi\varepsilon_0 r}$, $\vec{A} = \frac{B}{2}(-y, x, 0) \implies \vec{B} = (0, 0, B)$

$$H = \frac{1}{2m_e}\left[\left(p_x - \frac{eB}{2}y\right)^2 + \left(p_y + \frac{eB}{2}x\right)^2 + p_z^2\right] - \frac{e^2}{4\pi\varepsilon_0 r}$$

$$= \underbrace{\frac{p^2}{2m_e} - \frac{e^2}{4\pi\varepsilon_0 r}}_{H_{hyd}\,(B=0)} + \underbrace{\frac{eB}{2m_e}(xp_y - yp_x)}_{\text{paramagnetic}} + \underbrace{\frac{e^2B^2}{8m_e}(x^2+y^2)}_{\text{diamagnetic}}$$

Figure out what each term is doing

$$\frac{eB}{2m_e}(xp_y - yp_x) = \frac{e\hbar}{2m_e}\frac{L_z}{\hbar}B = \mu_B \underbrace{m}_{\text{azimuthal quan. \#}} B \qquad \text{Zeeman}$$

$\mu_0/2$

Typical size $\frac{\mu_B}{\hbar} \simeq 2\pi\ 14\ \text{GHz}/T = 2\pi\ 14\ \text{MHz}\ /(10\ \text{Gauss})$

Typical size $\frac{e^2B^2}{8m_e}(x^2+y^2) \sim \frac{e^2}{8m_e}B^2 a_0^2 n^4 \sim 10^{-29}\,J\left(\frac{B}{1T}\right)^2 n^4$

Convert to frequency by $1/h$ $\sim 15\ \text{kHz}\left(\frac{B}{1T}\right)^2 n^4 \implies$ (high n are easily perturbed)

In more complicated atoms, the Zeeman splittings can have substantial contribution from nucleus giving smaller result.

Example 2) $\varphi = \frac{e}{4\pi\varepsilon_0 r}$ $\vec{A} = -\frac{E_m}{\omega}(0, 0, \cos(kx-\omega t))$

Propagation direction of plane wave? Polarization?

Find E & B plane wave

$\vec{E} = -\frac{\partial \vec{A}}{\partial t} = E_m(0, 0, \sin(kx-\omega t))$ $\vec{B} = -\frac{E_m k}{\omega}(0, \sin(kx-\omega t), 0)$

$\vec{E}\times\vec{B} = \frac{E_m^2}{c}\left(\sin^2(kx-\omega t), 0, 0\right)$

If $E_m \ll$ E-field in atom

$H \cong \frac{p^2}{2m} - \frac{e^2}{4\pi\varepsilon_0 r} - \frac{E_m e}{m\omega} p_z \cos(kx-\omega t)$ <u>Velocity gauge</u>

In many situations, the wavelength of the light is much larger than the size of the atom

$\cos(kx-\omega t) = \underbrace{\cos(\omega t)}_{\text{dipole}} - \underbrace{kx\sin(\omega t)}_{\text{quadrupole}} \dots$

This is why dipole transition (example $1s \to 3p$) is typically much stronger than quadrupole transition (example $1s \to 3d$).

Gauge transformation can't change physics $\vec{A} \to \vec{A} + \vec{\nabla} f$

$\varphi \to \varphi - \frac{\partial f}{\partial t}$

$\vec{B} = \vec{\nabla}\times(\vec{A} + \vec{\nabla} f) = \vec{\nabla}\times\vec{A}$ ✓

$\vec{E} = -\vec{\nabla}\varphi - \frac{\partial \vec{A}}{\partial t} = -\vec{\nabla}\varphi + \nabla\frac{\partial f}{\partial t} - \frac{\partial \vec{A}}{\partial t} - \frac{\partial}{\partial t}\vec{\nabla} f = -\vec{\nabla}\varphi - \frac{\partial \vec{A}}{\partial t}$ ✓

Choose $f = \frac{E_m z}{\omega}\cos(\omega t) \to \vec{A} = -\frac{E_m}{\omega}(0, 0, \cos(\omega t - kx) - \cos(\omega t))$

$\varphi = E_m z \sin(\omega t)$

For $\lambda \gg$ size of atom $\vec{A} \simeq 0$

$H = \frac{p^2}{2m} - \frac{e^2}{4\pi\varepsilon_0 r} - e E_m z \sin(\omega t)$ <u>Length gauge</u>

Remember the approximation that goes into it!

How to know when the laser is strong? The intensity of light (units W/m^2) and frequency play role

$I = \frac{1}{2}\varepsilon_0 E_m^2 c$ $\qquad E_m = \sqrt{\frac{2I}{\varepsilon_0 c}}$

S Ghimire et al Nat Phys 7 138 (2011) had $E_m = 0.6\ V/\text{Å}$

$I = \frac{1}{2}\, 8.85\times10^{-12}(0.6\times10^{10})^2\, 3\times10^8\ W/m^2 = 4.8\times10^{16}\ W/m^2 = 4.8\times10^{12}\ W/cm^2$

(nowhere near best I)

$\lambda = 3.25\ \mu m \Rightarrow f = c/\lambda = 9.2\times10^{13}\ Hz \Rightarrow \omega = 2\pi f = 5.8\times10^{14}\ s^{-1}$

Important concept is quiver energy and excursion amplitude

$\ddot{x} = \frac{eE_m}{m_e}\cos(\omega t) \Rightarrow \dot{x} = \frac{eE_m}{\omega m_e}\sin(\omega t) \Rightarrow x = -\frac{eE_m}{m_e\omega^2}\cos(\omega t)$

Excursion amplitude $= \frac{eE_m}{m_e\omega^2} = 3.1\times10^{-9}\ m = 3.1\ nm$

Quiver energy $= \frac{m_e}{2}\left(\frac{eE_m}{\omega m_e}\right)^2 \underbrace{\frac{1}{2}}_{\text{avg of }\sin^2} = \frac{1}{m_e}\left(\frac{eE_m}{2\omega}\right)^2 = 7.5\times10^{-19}\ J = 4.7\ eV$

Ponderomotive energy, Ponderomotive potential

The energy of 1 photon $E = \frac{hc}{\lambda} = 6.12\times10^{-20}\ J = 0.38\ eV$

At this photon energy, 10+ photons are needed to ionize depending on the atom type.

Example 1: Laser wake field acceleration

Short, high intensity laser pulse pushes electrons out of region moving at $v \sim c$. Electrons pulled into wake can accelerate to GeV+ energies. Why electrons pushed out?

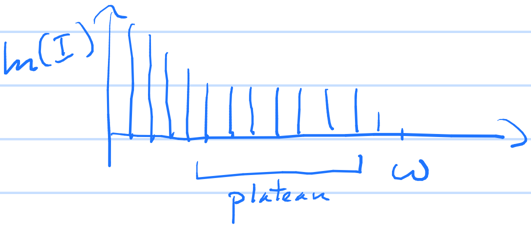
Example 2: High harmonic generation

At high intensities, the material will emit photons at frequencies $1\omega, 3\omega, 5\omega, \ldots$ (for symmetric potentials)

Why only odd for symmetric potentials?

$$\ddot{x} = -\omega^2 x - C x^3 + \alpha \sin(\omega t)$$

$$x = x_1 \sin(\omega t) + x_3 \sin(3\omega t) + x_5 \sin(5\omega t) \ldots$$



Cutoff $\sim I_p + 3.17\, U_p$

↳ ponderomotive energy

3 step model: 1) Tunnel out, 2) Free motion, 3) return to nucleus + emit photon.

After tunnel $v(t) = v_Q \sin(\omega t) + v_0 = v_Q\left[\sin(\omega t) + \frac{v_0}{v_Q}\right]$

$$x(t) = -\frac{v_Q}{\omega}\cos(\omega t) + \frac{v_Q}{\omega} + v_0 t = \frac{v_Q}{\omega}\left[1 - \cos(\omega t) + \frac{v_0}{v_Q}\omega t\right]$$

Find $v(t)$ when $x(t) = 0$. Maximum is when $v_0/v_Q \simeq -0.28$

$v(t) \simeq 1.265\, v_Q \Rightarrow$ $KE \simeq 3.2\, U_p$ Why add I_p to this?

Example 3: Above threshold ionization (ATI)

When laser intensity is high, atoms/molecules/solids can absorb many more photons than needed to ionize the atom.

Hydrogen atom + 1eV photons $\Rightarrow$ ionization with 14, 15, 16... photons

Electron energy $= nhf - I_p > 0$ $\quad n > I_p/hf$