Optically polarized atoms

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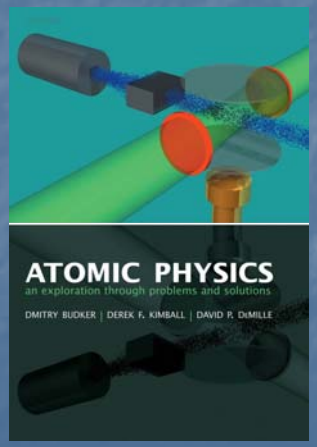
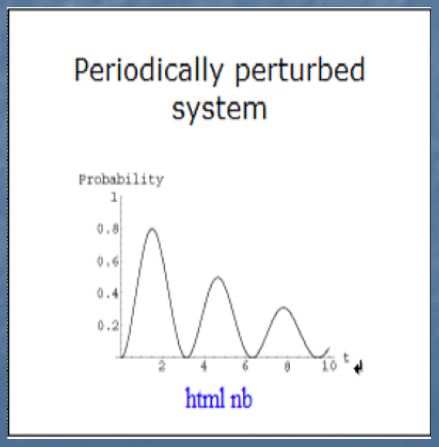
Chapter 5: Atomic transitions

- Preliminaries and definitions
  - Transition amplitude
  - Transition probability
  - Analysis of a two-level problem

See also:



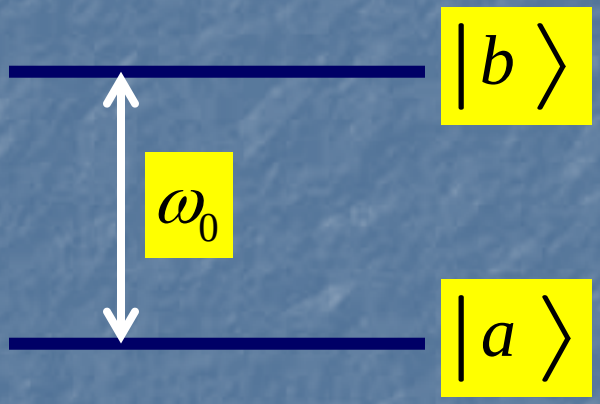
Problem 3.1



http://socrates.berkeley.edu/~budker/Tutorials/

Periodic perturbation

Two-level system



$$\mathbf{H} = \begin{pmatrix} 0 & V(t) \\ V^*(t) & \omega_0 \end{pmatrix}$$

$$V(t) = V_0 e^{i\omega t}$$

Initial Condition:

$$|\psi(0)\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Solving the problem…

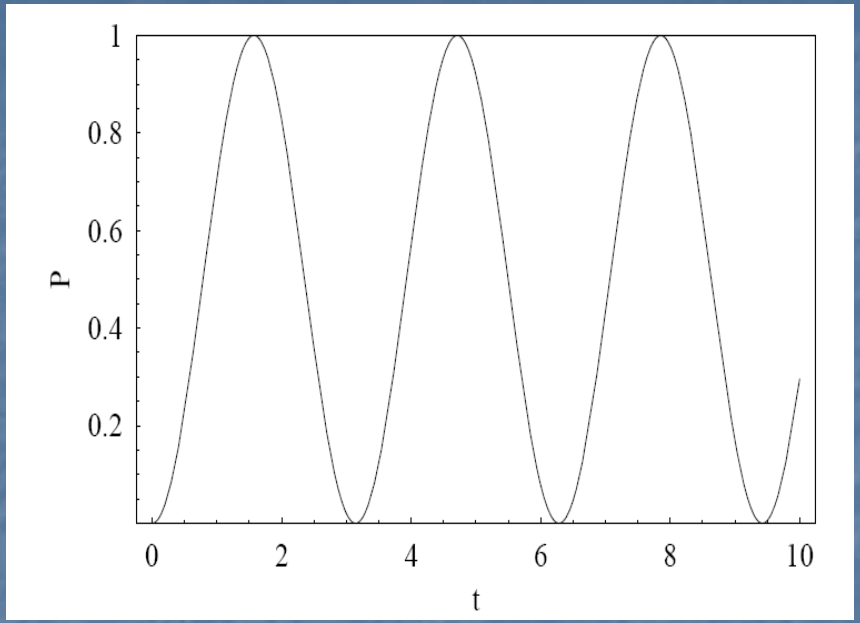
- There are many ways to solve for the probability of finding the system in either of the two states, including
  - Solve time-dependent Schrödinger equation
  - Make a unitary transformation to get rid of time dependence of the perturbation (this is equivalent to going into "rotating frame")
  - Solve the Liouville equation for the density matrix
- We will discuss all this in due time, but let us skip to the results for now…

P – probability of finding system in the upper state

$$\Delta = \omega - \omega_0 = 0$$

$$\Gamma = 0$$

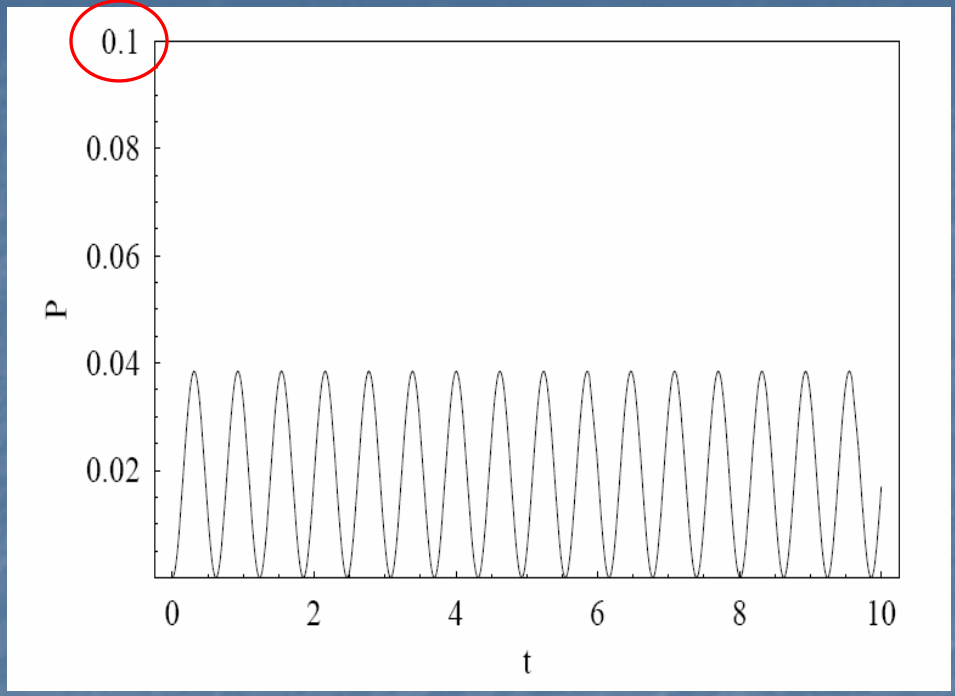
$$V_0 = 1$$



- Maximal-amplitude sinusoidal oscillations
- $P=\sin^2(V_0 t)=[1-\cos(\Omega_R t)]/2$; $\Omega_R=2V_0$ - Rabi frequency
- At small $t \Rightarrow P \propto t^2 \Rightarrow$ an interference effect (amplitudes from different dt add)
- Stimulated emission and stimulated absorption

P – probability of finding system in the upper state

$$\Delta = \omega - \omega_0 = 10$$
$$\Gamma = 0$$
$$V_0 = 1$$



- Non-maximal-amplitude sinusoidal oscillations
- Oscillation frequency: $\approx|\Delta|$
- For the cases where always P(t)<<1 :

$$P(t) = |b(t)|^2 = \frac{(2V_0)^2}{\Delta^2} \sin^2\left(\frac{\Delta t}{2}\right).$$

General solution for any Δ (Γ=0)

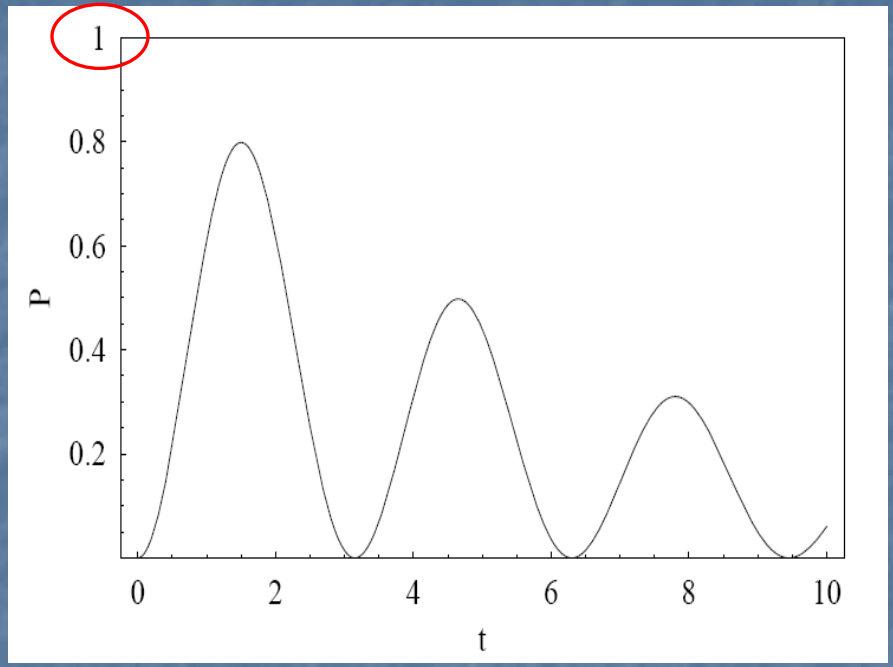
$$P(t) = \frac{(2V_0)^2}{(2V_0)^2 + \Delta^2} \sin^2 \left(\frac{1}{2} \left[(2V_0)^2 + \Delta^2 \right]^{1/2} t \right) .$$

Including the effect of relaxation

$$\Delta = \omega - \omega_0 = 0$$

$$\Gamma = 0.3$$

$$V_0 = 1$$



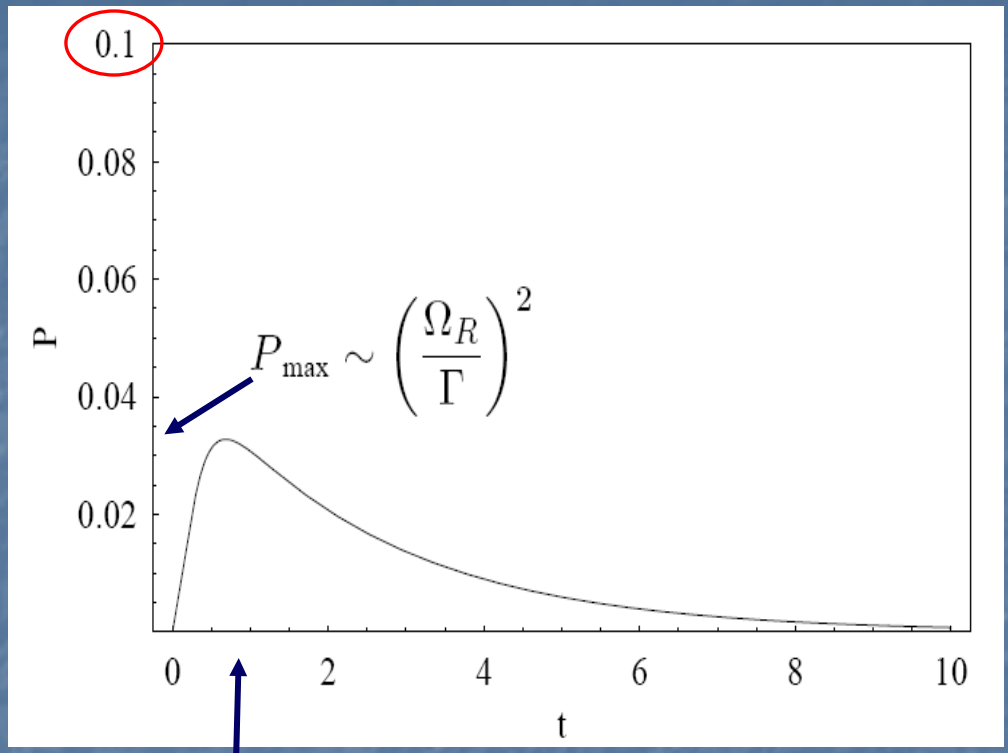
- Decay to unobserved levels (outside the system)
- Damped oscillations

Including the effect of relaxation

$$\Delta = \omega - \omega_0 = 0$$

$$\Gamma = 10$$

$$V_0 = 1$$



- Overdamped regime – no oscillations
- This occurs for $\Gamma > 2\Omega_R$
- The system behaves as if there is no relaxation for small *t*
- General analytical formula :

$$P(t) = \frac{(2V_0)^2 e^{-\Gamma t/2}}{(2V_0)^2 + \Delta^2 + \Gamma^2/4} \sin^2\left(\frac{t}{2}\sqrt{(\Delta + \Gamma/2)^2 + (2V_0)^2}\right)$$

Selection rules

- Certain quantities must remain conserved in a transition
- An easy way to think about it is the photon picture
- Conserved quantities: energy, momentum, total angular momentum, …
- We have many angular momenta for atoms:

L S J I F

- Forget **I** ⇒ J=**F** for now (to make life easier)
- For electric-dipole (E1) transitions, $\mathbf{J}_{phot}$= $\mathbf{S}_{phot}$=1; $\mathbf{L}_{phot}$=0
- Adding or subtracting angular momentum one changes angular momentum of a system by 0,+1, or -1

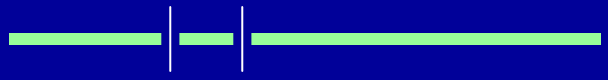
$$\Delta J = J_f - J_i = 0, \pm 1.$$

- Also, 0⟶0 transitions are forbidden
- Generally, we have triangle rule

Entertaining Interlude: cutting a stick

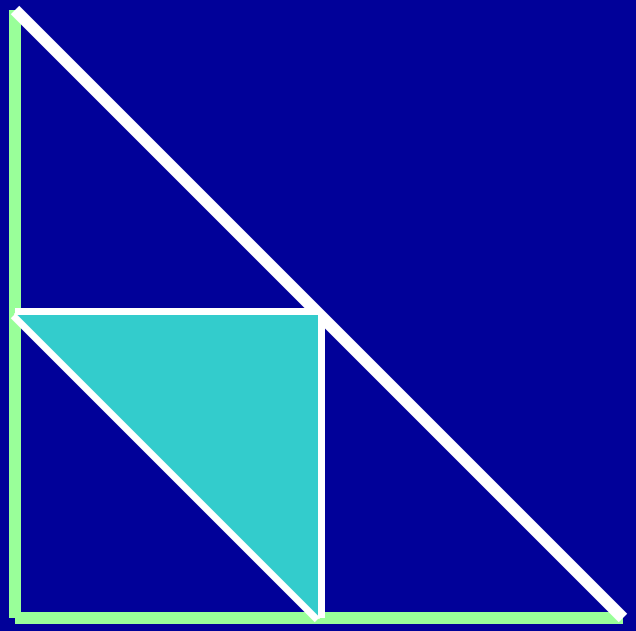
or getting to know the triangle rule

A stick is randomly cut into three



Q. What is the probability that one can make a triangle out of the resultant sticks ?

A. 1/4



Selection rules

Q: What changes when **J** changes, **L**, **S**, or both ?

- A: it is **L** that changes ⇒ orbital rearrangement
- In classical electrodynamics, emission and absorption have to do with accelerating charges
- Additional selection rules (good to the extent L,S are good quantum #s):

$$\Delta L = 0, \pm 1.$$

$$L_i + L_f \geq 1.$$

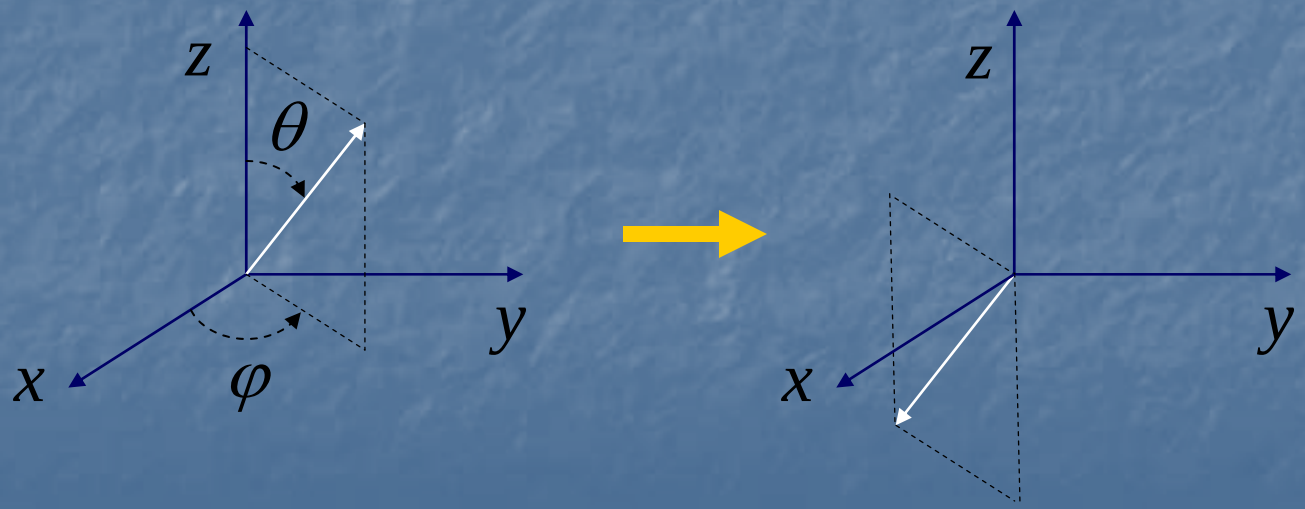
$$\Delta S = 0.$$

- Another form of the

  0⟶0 transitions are forbidden rule

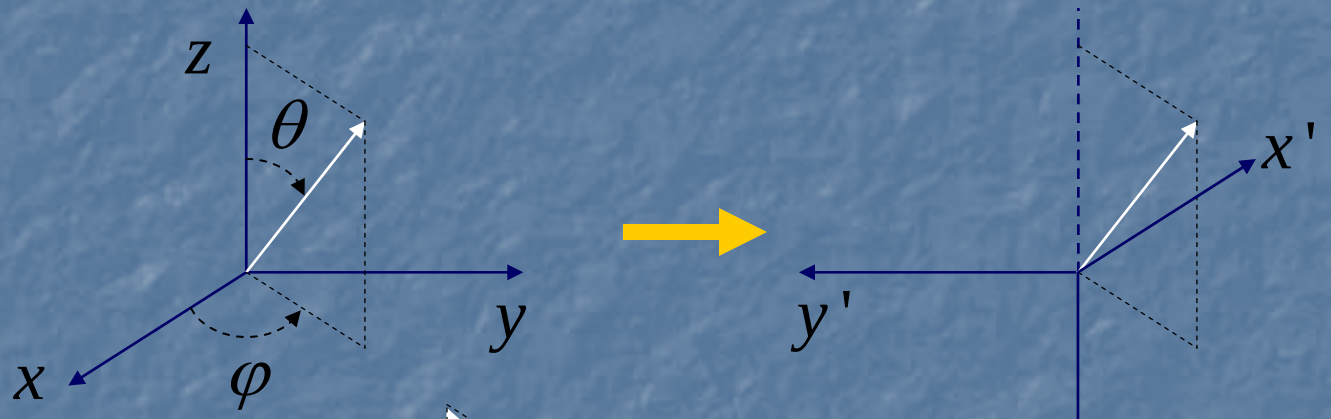
Parity of atomic states

- Spatial inversion (P) : $x \to -x, y \to -y, z \to -z$
- Or, in polar coordinates : $r \to r, \theta \to \pi - \theta, \varphi \to \varphi + \pi$

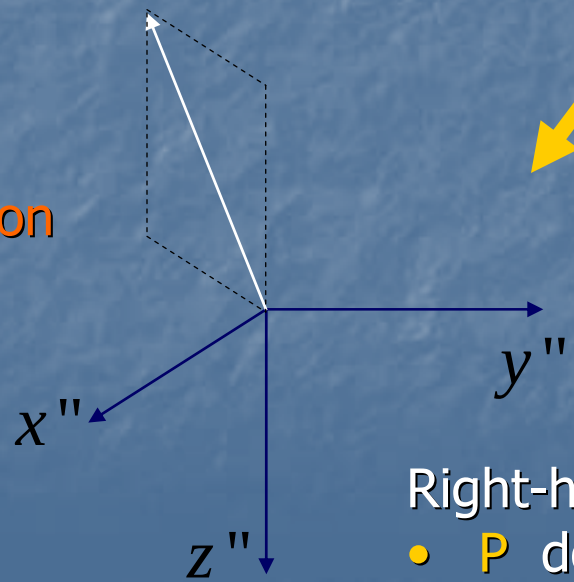


Parity of atomic states

- It might seem that P is an operation that may be reduced to rotations
- This is **NOT** the case
- Let's see what happens if we invert a coordinate frame :



- Now apply a π rotation



Right-handed frame ⇒ left handed

- P does **NOT** reduce to rotations !

Parity of atomic states

- An amazing fact : atomic Hamiltonian is rotationally invariant but **is NOT P-invariant**
- We will discuss parity nonconservation effects in detail later on in the course…

Parity of atomic states

- In hydrogen, the electron is in centro-symmetric nuclear potential
- In more complex atoms, an electron sees a more complicated potential
- If we approximate the potential from nucleus and other electrons as centro-symmetric (and not parity violating) , then :

$$\psi_{nlm}(r,\theta,\varphi) = R_{nl}(r)Y_{lm}(\theta,\varphi).$$

Wavefunctions in this form
are automatically of certain parity :

$$\psi_{nlm} \xrightarrow{P} (-1)^l \psi_{nlm}$$

This is because:

$$Y_{lm}(\pi-\theta,\varphi+\pi) = (-1)^l Y_{lm}(\theta,\varphi)$$

- Since multi-electron wavefunction is a properly antisymmetrized product of wavefunctions for each electron, parity of a multi-electron state is a product of parities for each electron:

$$(-1)^{\sum_i l_i}$$

Comments on multi-electron atoms

- Potential for individual electrons is NOT centrosymmetric
- Angular momenta and parity of individual electrons are not exact notions (configuration mixing, etc.)
- But for the system of all electrons, total angular momentum and parity are good !
- Parity of a multi-electron state:

$$(-1)^{l_1}(-1)^{l_2}\ldots(-1)^{l_n}$$

W A R N I N G

~~$(-1)^{L}$~~

Parity of atomic states

A bit of formal treatment…

- Hamiltonian is P-invariant (ignoring PNC) : $P^{-1}\mathbf{H}P=\mathbf{H}$
- $\Rightarrow$ spatial-inversion operator commutes with Hamiltonian :

$$[P,\mathbf{H}]=0$$

- $\Rightarrow$ stationary states are simultaneous eigenstates of **H** and P
- What about eigenvalues (p; $P\psi=p\psi$) ?
- Note that doing spatial inversion twice brings us back to where we started
- $P^2\,\psi=P(P\,\psi)=P(p\psi)=p(P\psi)=p^2\,\psi$. This has to equal $\psi \Rightarrow p^2=1 \Rightarrow p=\pm 1$
- p=1 – even parity; p=-1 – odd parity

Back to dipole transitions

- Transition amplitude : $\langle \psi_2 | \mathbf{d} | \psi_1 \rangle$, where $\mathbf{d} = e \cdot \mathbf{r}$ is the dipole operator
- For multi-electron atoms dipole operator is sum over electrons : $\mathbf{d} = \sum_i \mathbf{d}_i$
- However, the operator changes at most one electron at a time, so for pure configurations, transitions are only allowed between states different just by one electron, for example (in Sm) :

$$(Xe)4f^6 6s6p \longrightarrow (Xe)4f^6 6s7s$$

$$(Xe)4f^6 6s6p \longrightarrow (Xe)4f^6 7p6p$$

$$(Xe)4f^6 6s6p \not\longrightarrow (Xe)4f^6 7p7s$$

Parity selection rule

- Transition amplitude :

$$\langle \psi_2 | \mathbf{r} | \psi_1 \rangle = \int d^3 r \, (\psi_2 \mathbf{r} \psi_1)$$

Odd under P

- This means that for the amplitude not to vanish, the product

$$(\psi_2 \psi_1)$$

must also be P-odd

➢ Initial and final states must be of **opposite parity**

Higher-multipole radiative transitions

- If electric-dipole-transition (E1) selection rules not satisfied ⇒

forbidden transitions

- E1 are due to the electric-dipole Hamiltonian: $H_d = -\mathbf{d}\cdot\mathbf{E}$
- In analogy, there are magnetic-dipole transitions due to: $H_m = -\boldsymbol{\mu}\cdot\mathbf{B}$
- Also, there are electric-quadrupole transitions due to:

$$H_Q = -\frac{1}{6}\sum_{i,j} Q_{ij}\frac{\partial E_j}{\partial x_i}.$$

- Each type of transitions has associated selection rules

Magnetic-dipole transitions

- Let us estimate the ratio of the transition matrix elements for M1 and E1
- A typical atomic electric-dipole moment is ea
- A typical atomic magnetic-dipole moment is μ_0
- Transition probability:

$$\propto \frac{W(M1)}{W(E1)} \sim \left(\frac{\mu_0}{ea}\right)^2 = \left(\frac{\frac{e\hbar}{2mc}}{e\frac{\hbar^2}{me^2}}\right)^2 = \left(\frac{e^2}{2\hbar c}\right)^2 = \left(\frac{\alpha}{2}\right)^2 \sim 10^{-5}$$

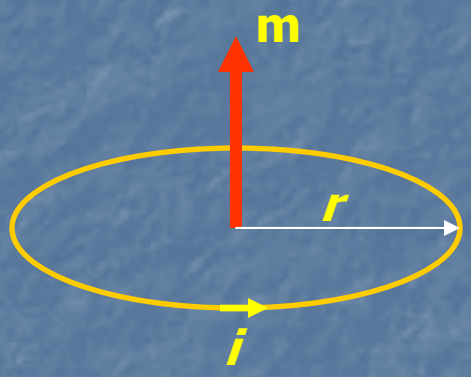
Magnetic-dipole transitions

- What are the M1 selection rules ?
- Imagine a transition between levels for which E1 angular-momentum selection rules are satisfied, but parity rule is not
- Notice: **m** is a pseudo-vector (= axial vector), i.e. it is invariant with respect to spatial inversion. Imagine a current loop:

$$\mathbf{m} \equiv \frac{1}{2c}\int \mathbf{r}\times\mathbf{j}(\mathbf{r})\,d^3r = \frac{i\left(\pi r^2\right)\mathbf{n}}{c}$$

P-odd P-odd

P-even !



M1 transitions occur between states of same parity

Magnetic-dipole transitions

Important M1 transitions occur :

- between Zeeman sublevels of the same state: NMR, optical-pumping magnetometers, etc.
- between hyperfine-structure levels: atomic clocks, the 21-cm line

This horn antenna, now displayed in front of the Jansky Lab at NRAO in Green Bank, WV, was used by Harold Ewen and Edward Purcell, then at the Lyman Laboratory of Harvard University, in the first detection of the 21 cm emission from neutral hydrogen in the Milky Way. The emission was first detected on March 25, 1951.
See: http://www.nrao.edu/whatisra/hist_ewenpurcell.shtml

Some other multipole transitions

Electric-quadrupole (E2) transitions

$$\begin{aligned} \Delta J &= 0, \pm 1, \pm 2 \qquad J + J' \geq 2, \\ \Delta M_J &= 0, \pm 1, \pm 2 \end{aligned}$$

No parity change !

With LS coupling, we also have

$$\begin{aligned} \Delta L &= 0, \pm 1, \pm 2 \qquad L + L' \geq 2 \\ \Delta S &= 0, \end{aligned}$$

This can be continued (E3,M2,…)

How to calculate E1 transition probability

- Imagine classical oscillating dipole **d** interacting with resonant linearly-polarized electric field **E**
- The rate of absorption of energy by the dipole is

$$\propto \left(\mathbf{d}\cdot \mathrm{E}\right)^2 = d^2 E^2 \cos^2\theta$$

"Dynamic factors" "Geometric factor"

- We have something similar in quantum mechanics: transition probability between the initial and final state is proportional to:

$$\left|\langle \xi' J' M' | \mathbf{E}\cdot\mathbf{d} | \xi J M\rangle\right|^2 = \langle \xi' J' M' | \mathbf{E}\cdot\mathbf{d} | \xi J M\rangle \langle \xi' J' M' | \mathbf{E}\cdot\mathbf{d} | \xi J M\rangle^*.$$

How to calculate E1 transition probability

- Let us recall how this comes about…
- For single-electron atom, neglecting nuclear spin

$$H = \frac{1}{2m}\left[\mathbf{p} + \frac{e}{c}\mathbf{A}(\mathbf{r},t)\right]^2 - \frac{Ze^2}{r}$$

- Can this be simplified ?
- Let's relate the light electric field and the vector potential $\mathcal{E}_0 \sim \frac{1}{c}\frac{\partial A}{\partial t} \sim \frac{\omega}{c}A$
- We can relate electron momentum to atomic electric field; this shows that if the light field is much weaker than the atomic field, the term quadratic in **A** can be neglected; this is usually the case (except modern ultra-short laser pulses)

How to calculate E1 transition probability

- In this approximation and neglecting electron spin :

$$H_0 + H_1 = \frac{p^2}{2m} - \frac{Ze^2}{r} + \frac{e}{2mc}(\mathbf{p}\cdot\mathbf{A} + \mathbf{A}\cdot\mathbf{p})$$

Under the Coulomb gauge $\nabla \cdot \mathbf{A} = 0$ we have

$$\begin{aligned}(\mathbf{A}\cdot\mathbf{p})\,\psi &= -i\hbar\mathbf{A}\cdot\nabla\psi \\ &= -i\hbar\left[\nabla\cdot(\mathbf{A}\psi) - \psi(\nabla\cdot\mathbf{A})\right] \\ &= (\mathbf{p}\cdot\mathbf{A})\,\psi\end{aligned} \tag{5.25}$$

Thus the perturbation H_1 can be rewritten as

$$H_1 = \frac{e}{mc}\mathbf{p}\cdot\mathbf{A}. \tag{5.26}$$

For a quantized electromagnetic field the vector potential can be written as

$$\mathbf{A} = \sqrt{\frac{2\pi\hbar c^2}{V\omega}}\left[a\hat{\mathbf{E}}e^{i\mathbf{k}\cdot\mathbf{r}} + a^\dagger\hat{\mathbf{E}}^* e^{-i\mathbf{k}\cdot\mathbf{r}}\right] \tag{5.27}$$

where V is the volume of the box in which normalization of $\mathbf{A}$ is performed.

How to calculate E1 transition probability

- To calculate transition probability, take matrix elements of perturbation between combined states of light and atoms: $|\xi JM\rangle|n\rangle$
- For absorption, $n+1 \longrightarrow n$

$$\begin{aligned}
&\langle n|\langle \xi' J' M'|H_1|\xi JM\rangle|n+1\rangle \\
&\qquad \propto \langle n|\langle \xi' J' M'|a\mathbf{p}\cdot\hat{\mathbf{E}}e^{i\mathbf{k}\cdot\mathbf{r}} + a^\dagger \mathbf{p}\cdot\hat{\mathbf{E}}^* e^{-i\mathbf{k}\cdot\mathbf{r}}|\xi JM\rangle|n+1\rangle \\
&\qquad = \sqrt{n}\langle \xi' J' M'|\mathbf{p}\cdot\hat{\mathbf{E}}e^{i\mathbf{k}\cdot\mathbf{r}}|\xi JM\rangle,
\end{aligned}$$

- Here we used essential results from QED:
- These reflect the essential bosonic properties of light, and relate stimulated emission and absorption with spont. em.

$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$$
$$a|n\rangle = \sqrt{n}|n-1\rangle.$$

How to calculate E1 transition probability

$$\begin{aligned}
&\langle n|\langle \xi' J' M'|H_1|\xi J M\rangle|n+1\rangle \\
&\qquad \propto \langle n|\langle \xi' J' M'|a\mathbf{p}\cdot\hat{\mathbf{E}}e^{i\mathbf{k}\cdot\mathbf{r}} + a^\dagger \mathbf{p}\cdot\hat{\mathbf{E}}^* e^{-i\mathbf{k}\cdot\mathbf{r}}|\xi J M\rangle|n+1\rangle \\
&\qquad = \sqrt{n}\langle \xi' J' M'|\mathbf{p}\cdot\hat{\mathbf{E}}e^{i\mathbf{k}\cdot\mathbf{r}}|\xi J M\rangle,
\end{aligned}$$

- Next, we apply the Dipole Approximation : $e^{i\mathbf{k}\cdot\mathbf{r}} \approx 1.$
- and make use of the Heisenberg eqn: $[\mathbf{r}, H_0] = \frac{i\hbar}{m}\mathbf{p}$

Interlude: the Heisenberg Eqn.

- Classical momentum: $$\mathbf{p} = m\mathbf{v} = m\frac{d\mathbf{r}}{dt}$$

- In QM, time derivative of any operator is given by commutator with the Hamiltonian

$$\frac{d\mathbf{r}}{dt} = \frac{i}{\hbar}\left[H, \mathbf{r}\right] = \frac{i}{\hbar}\left(H\mathbf{r} - \mathbf{r}H\right)$$

$$\mathbf{p} = m\frac{d\mathbf{r}}{dt} = \frac{im}{\hbar}\left[H, \mathbf{r}\right]$$

How to calculate E1 transition probability

- With this we have :

$$\langle \xi' J' M' | \mathbf{p} \cdot \hat{\mathbf{E}} | \xi J M \rangle = \frac{m}{i\hbar} \langle \xi' J' M' | \left(\mathbf{r} H_0 - H_0 \mathbf{r} \right) \hat{\mathbf{E}} | \xi J M \rangle$$
$$= \frac{m}{i\hbar e} \left(E_J - E_{J'} \right) \langle \xi' J' M' | \mathbf{d} \cdot \hat{\mathbf{E}} | \xi J M \rangle$$

- We see that for absorption, amplitude is $\propto$ $\langle \xi' J' M' | \hat{\mathbf{E}} \cdot \mathbf{d} | \xi J M \rangle .$

- while for emission, amplitude is $\propto$ $\langle \xi J M | \hat{\mathbf{E}}^* \cdot \mathbf{d} | \xi' J' M' \rangle .$

- Scalar product of vectors can be written as

$$\hat{\mathbf{E}} \cdot \mathbf{d} = \sum_q \hat{E}^q d_q .$$

How to calculate E1 transition probability

- With this we have :

$$\langle \xi' J' M' | \hat{\mathbf{E}} \cdot \mathbf{d} | \xi J M \rangle = \sum_{q=-1}^{1} \hat{E}^q \langle \xi' J' M' | d_q | \xi J M \rangle .$$

- We next concentrate on the ME of the components of the dipole moment
- The dynamic and angular parts are separated using the all-important

Wigner-Eckart Theorem

$$\langle \xi' J' M' | d_q | \xi J M \rangle = (-1)^{J'-M'} \begin{pmatrix} J' & 1 & J \\ -M' & q & M \end{pmatrix} (\xi' J' \| d \| \xi J)$$

"3j symbol"

How to calculate E1 transition probability

- Wigner-Eckart Theorem

$$\langle \xi' J' M' | d_q | \xi J M \rangle = (-1)^{J'-M'} \begin{pmatrix} J' & 1 & J \\ -M' & q & M \end{pmatrix} (\xi' J' \| d \| \xi J)$$

"3j symbol"

Reduced matrix element

- Useful property :

$$(\xi' J' \| d \| \xi J) = (-1)^{J'-J} (\xi J \| d \| \xi' J')^*$$

3j symbols

- Represent the geometric part of transition amplitude
- Reduced matrix element – no reference to projections:

  dynamic part
- 3j symbols are standard functions in Mathematica™
- Contain selection rules for angular-momenta addition,

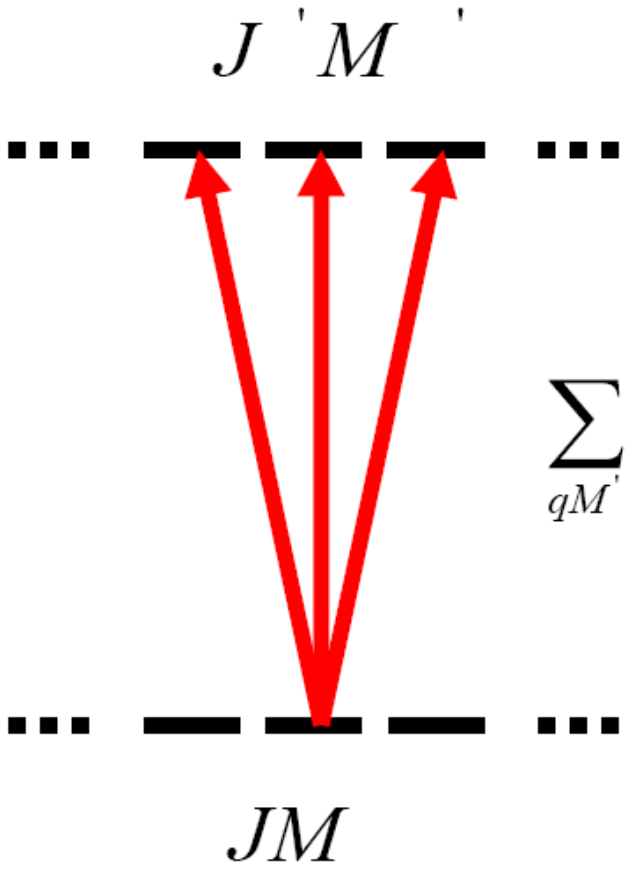
  including the triangular condition

$$|J-1| \leq J' \leq J+1$$

- and the projection rule

$$q + M - M' = 0.$$

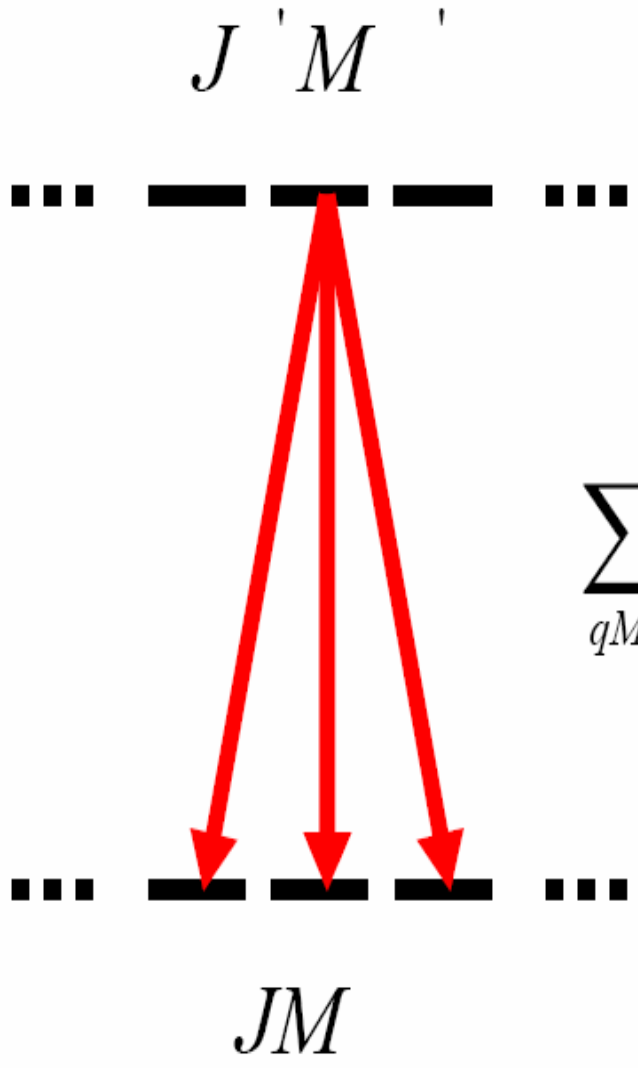
3j symbols: sum rules



$$\sum_{qM'} \left| \left\langle J'M' \middle| d_q \middle| JM \right\rangle \right|^2 = \frac{\left| \left\langle \xi' J' \middle\| d \middle\| \xi J \right\rangle \right|^2}{(2J+1)}$$

(a)

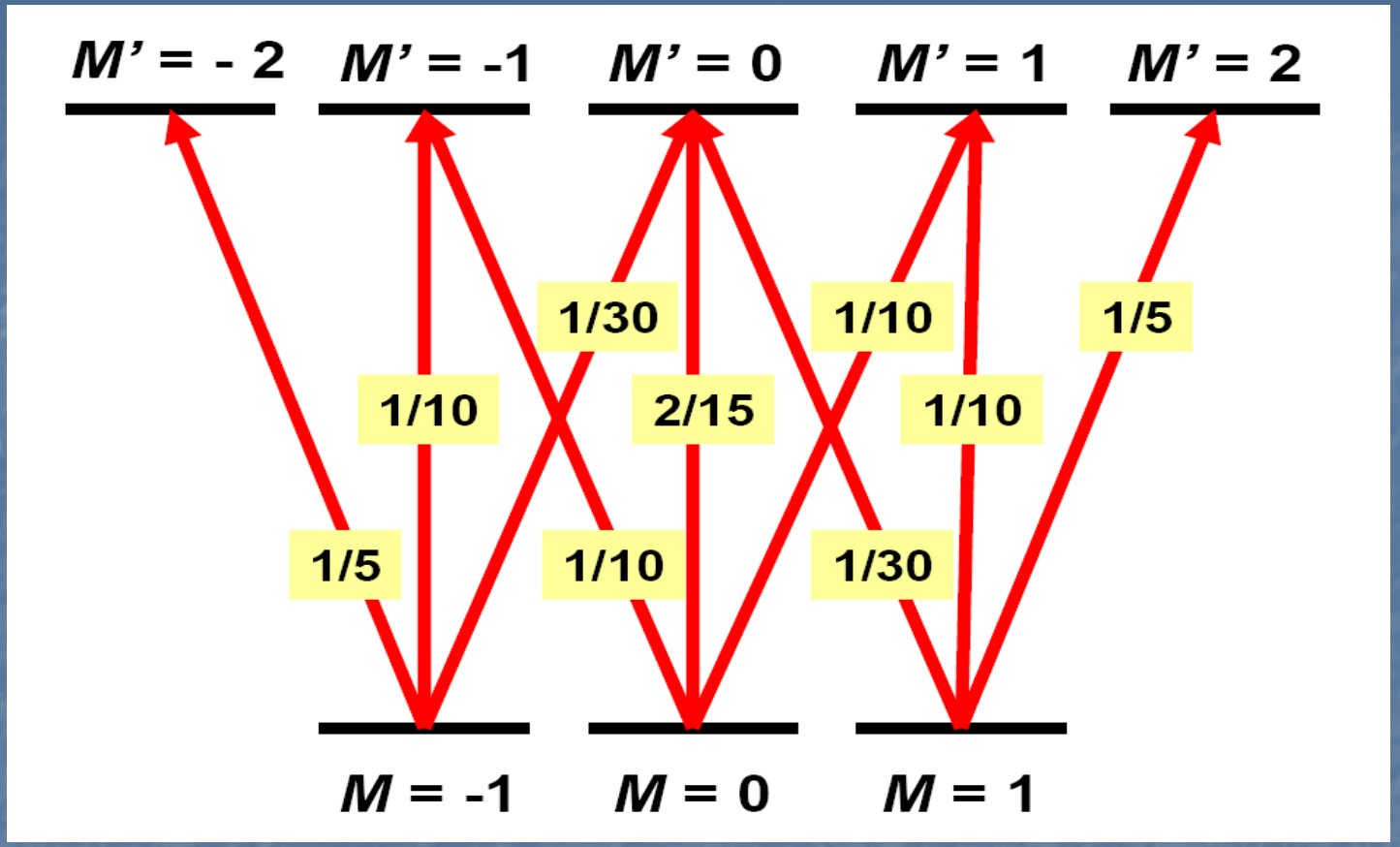
3j symbols: sum rules



$$\sum_{qM}\left|\left\langle JM\left|d_q\right|J'M'\right\rangle\right|^2=\frac{\left|\left\langle \xi J\left\|d\right\|\xi' J'\right\rangle\right|^2}{(2J'+1)}$$

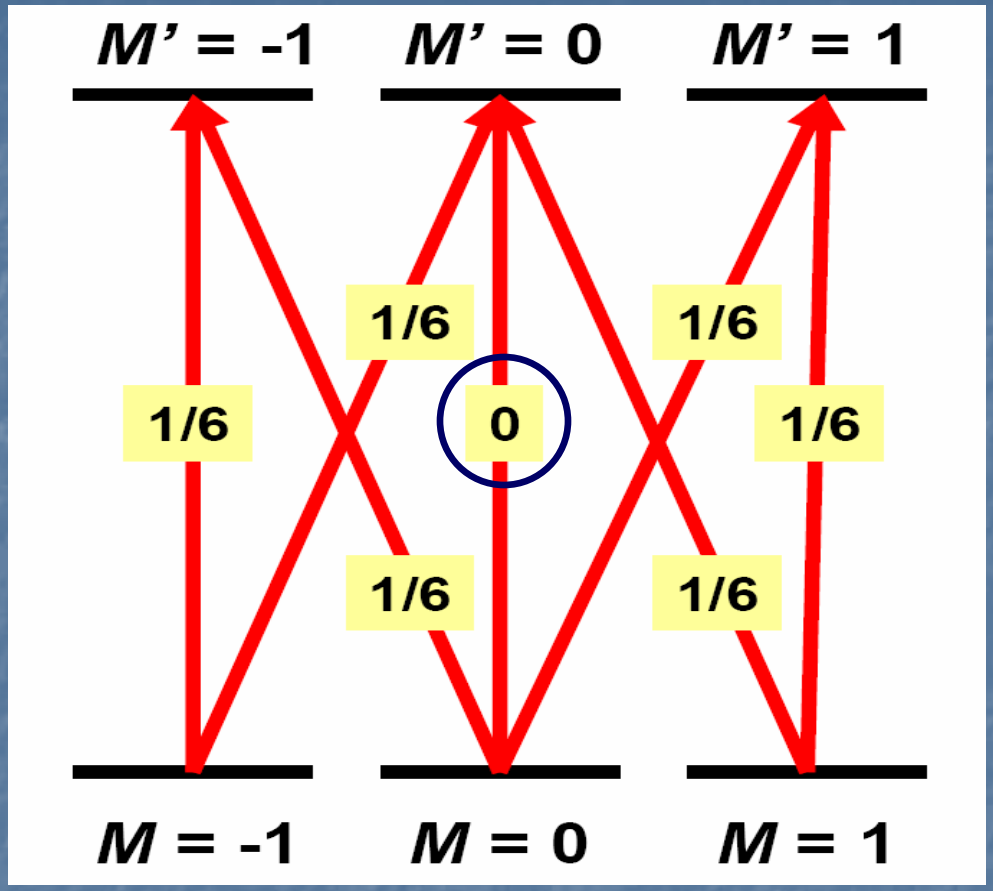
(b)

Relative transition strengths J=1⟶J'=2



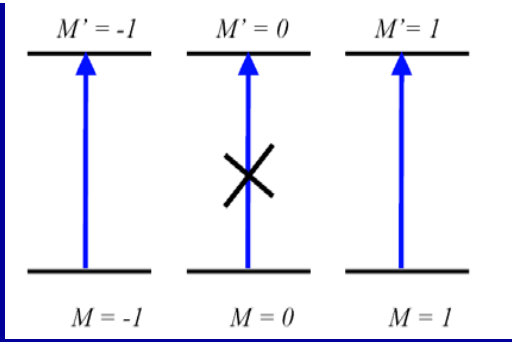
$$\sum_{qM'} \left| \left\langle J'M' \left| d_q \right| JM \right\rangle \right|^2 = \frac{\left| \left\langle \xi' J' \| d \| \xi J \right\rangle \right|^2}{(2J+1)}$$

Relative transition strengths J=1⟶J′=1



$$\sum_{qM'} \left| \left\langle J'M' \middle| d_q \middle| JM \right\rangle \right|^2 = \frac{\left| \left\langle \xi' J' \middle\| d \middle\| \xi J \right\rangle \right|^2}{(2J+1)}$$

Interlude: why is M=0⟶M′=0 transition forbidden for J=J′=1 ?



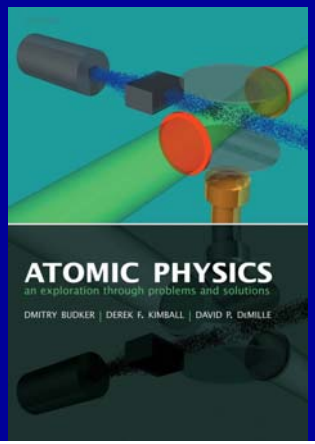
- J=1, J′=1, photon – vector "particles"
- Duality between q (or M) and polarization vector

M	Polarization vector
-1	$\propto \hat{x} - i\hat{y}$
0	$\propto \hat{z}$
$+1$	$\propto \hat{x} + i\hat{y}$

- Building final vector out of initial polarization vectors:

The only possibility: $\mathbf{E} \propto \mathbf{E}_1 \times \mathbf{E}_2.$

- =0 when both vectors are along **z**



Reduced matrix elements in LS coupling

- As far as LS coupling holds, we can make further simplifications; label states conspicuously : $|JM_J\rangle = |(LS)JM_J\rangle$
- Only **L** changes in E1 transitions

$$
\begin{aligned}
& (\xi'(L'S)J'\|d\|\xi(LS)J) \\
= \quad & (-1)^{L'+S+J+1}\sqrt{(2J+1)(2J'+1)}\begin{Bmatrix} L' & J' & S \\ J & L & 1 \end{Bmatrix}(\xi' L'\|d\|\xi L
\end{aligned}
$$

"6j symbol"

- Note: no mention of projections
- 6j symbols obey a number of triangular conditions

Triangular conditions for 6j symbols

$$\left\{ \begin{array}{ccc} L' & J' & S \\ J & L & 1 \end{array} \right\}$$

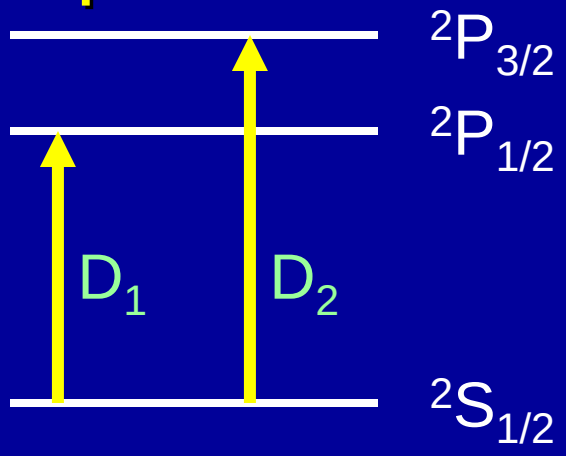
- Each of the following angular momenta must form a triangle:

$$\left\{ \begin{array}{ccc} * & * & * \\ \cdot & \cdot & \cdot \end{array} \right\}, \left\{ \begin{array}{ccc} \cdot & \cdot & * \\ * & * & \cdot \end{array} \right\}, \left\{ \begin{array}{ccc} * & \cdot & \cdot \\ \cdot & * & * \end{array} \right\}, \left\{ \begin{array}{ccc} \cdot & * & \cdot \\ * & \cdot & * \end{array} \right\}$$

- 6j symbols are real numbers
- 6j symbols are standard functions in Mathematica™
- Our discussion translates to hyperfine transitions

with $L \longrightarrow J$, $L' \longrightarrow J'$, $J \longrightarrow F$, $J' \longrightarrow F'$, $S=S' \longrightarrow I$

Example: alkali D lines



$$\begin{aligned}
&(\xi'(L'S)J'\|d\|\xi(LS)J) \\
= \;& (-1)^{L'+S+J+1}\sqrt{(2J+1)(2J'+1)}\left\{\begin{array}{ccc} L' & J' & S \\ J & L & 1 \end{array}\right\}(\xi'L'\|d\|\xi L
\end{aligned}$$

- Compare transition strengths :

$^2S_{1/2} \rightarrow {}^2P_{1/2}$ transition is

$$\begin{aligned}
&|(\xi' 1/2\|d\|\xi 1/2)|^2 \\
= \;& |(\xi'(L'=1,S=1/2)J'=1/2\|d\|\xi(L=0,S=1/2)J=1/2)|^2 \\
= \;& (-1)^{2(1+1/2+1/2+1)}\,4\left\{\begin{array}{ccc} 1 & 1/2 & 1/2 \\ 1/2 & 0 & 1 \end{array}\right\}^2 \times \\
& |(\xi' L'=1\|d\|\xi L=0)|^2 ,
\end{aligned}$$

for the $^2S_{1/2} \rightarrow {}^2P_{3/2}$ transition it is

$$\begin{aligned}
&|(\xi' 3/2\|d\|\xi 1/2)|^2 \\
= \;& |(\xi'(L'=1,S=1/2)J'=3/2\|d\|\xi(L=0,S=1/2)J=1/2)|^2 \\
= \;& (-1)^{2(1+1/2+1/2+1)}\,8\left\{\begin{array}{ccc} 1 & 3/2 & 1/2 \\ 1/2 & 0 & 1 \end{array}\right\}^2 \times \\
& |(\xi' L'=1\|d\|\xi L=0)|^2 .
\end{aligned}$$

- Evaluate :

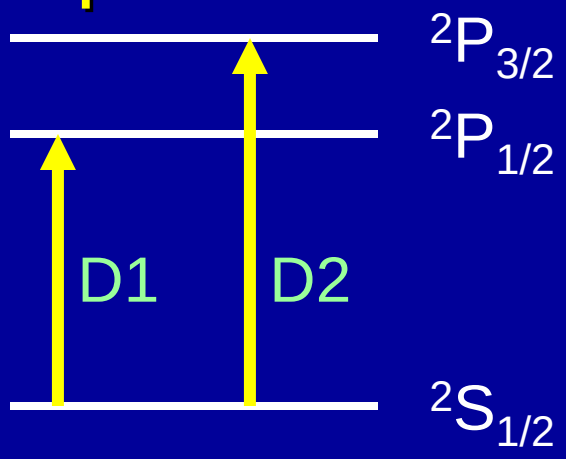
$$\left\{\begin{array}{ccc} 1 & 1/2 & 1/2 \\ 1/2 & 0 & 1 \end{array}\right\} = \frac{1}{\sqrt{6}}$$

$$\left\{\begin{array}{ccc} 1 & 3/2 & 1/2 \\ 1/2 & 0 & 1 \end{array}\right\} = -\frac{1}{\sqrt{6}}$$

$$\frac{|(\xi' 1/2\|d\|\xi 1/2)|^2}{|(\xi' 3/2\|d\|\xi 1/2)|^2} = \frac{1}{2}$$

- D2 is twice stronger than D1

Example: alkali D lines



- Reduced matrix elements can be extracted from lifetimes:

$$|(\xi' J' \| d \| \xi J)|^2 \frac{1}{2J'+1} \frac{4\omega_0^3}{3\hbar c^3} = \frac{1}{\tau}$$

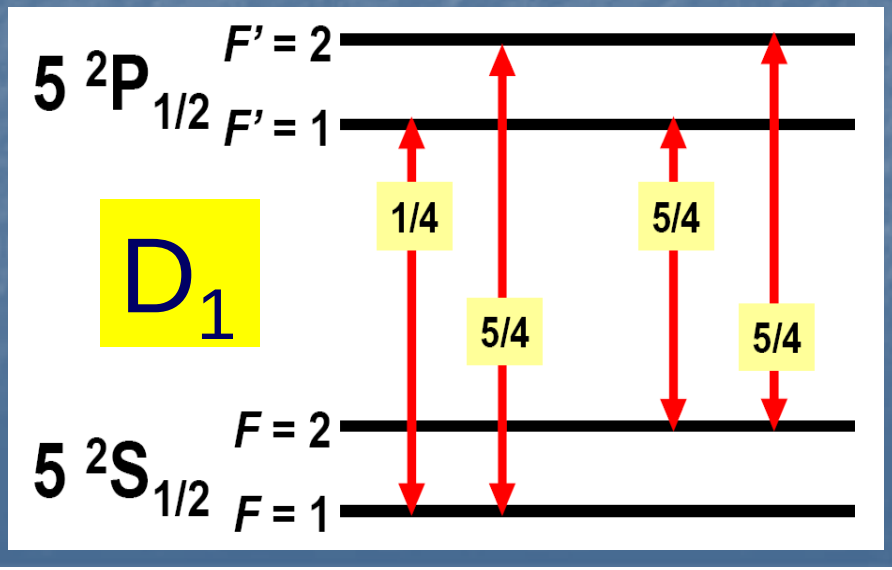
- Prediction (D_2 is twice stronger than D_1) confirmed by experiment :

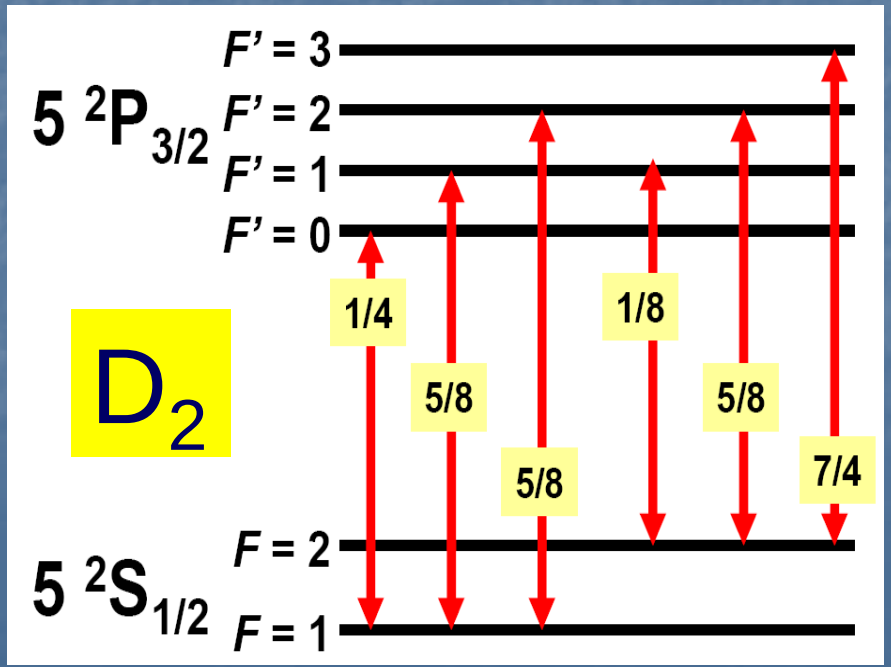
Alkali atom	$(J\|\|d\|\|J')$	numerical value	
		$(J\|\|d\|\|J')$	$\frac{\|(1/2\|\|d\|\|3/2)\|^2}{\|(1/2\|\|d\|\|1/2)\|^2}$
^{23}Na	$(1/2\|\|d\|\|3/2)$	$4.9847 ea_0$	2.0000
	$(1/2\|\|d\|\|1/2)$	$3.5246 ea_0$	
^{87}Rb	$(1/2\|\|d\|\|3/2)$	$5.978 ea_0$	1.996
	$(1/2\|\|d\|\|1/2)$	$4.231 ea_0$	
^{133}Cs	$(1/2\|\|d\|\|3/2)$	$6.3337 ea_0$	1.9807
	$(1/2\|\|d\|\|1/2)$	$4.5003 ea_0$	

Hyperfine structure

$$(\xi'(J'I)F'\|d\|\xi(JI)F)$$
$$= (-1)^{J'+I+F+1}\sqrt{(2F+1)(2F'+1)}\left\{\begin{array}{ccc} J' & F' & I \\ F & J & 1 \end{array}\right\}(\xi' J'\|d\|\xi J)$$

- Line strength : $S(FF') = |(\xi'(J'I)F'\|d\|\xi(JI)F)|^2$
- Examples: alkali atoms with *I*=3/2 (^{7}Li, ^{23}Na, ^{39}K, ^{41}K, ^{87}Rb)





Hyperfine structure

- Normalization:

$$\sum_F S(FF') = \frac{2F'+1}{2J'+1}, \qquad \sum_{F'} S(FF') = \frac{2F+1}{2J+1}$$

- To compare line strengths for different manifolds, need to account for the difference in reduced ME
- Combining formulae for fine and hyperfine structure:

$$\begin{aligned}
&(\xi'((L'S)J'I)F'\|d\|\xi((LS)JI)F) \\
= \quad &(-1)^{L'+S+J+1}\sqrt{(2J+1)(2J'+1)}\left\{\begin{array}{ccc} L' & J' & S \\ J & L & 1 \end{array}\right\} \\
&(-1)^{J'+I+F+1}\sqrt{(2F+1)(2F'+1)}\left\{\begin{array}{ccc} J' & F' & I \\ F & J & 1 \end{array}\right\}(\xi L'\|d\|\xi L)
\end{aligned}$$

Multipole transitions for Segway™ riders

- As opposed to pedestrians
- In the E1 approximation, we neglect spatial variation of light field over the size of an atom and set $\exp(\pm i\mathbf{k}\cdot\mathbf{r}) = 1$
- This is because:

$$kr = \frac{\omega}{c} r \sim \frac{\omega}{c} a_0 \sim \frac{Ry}{\hbar c} \cdot a_0 = \frac{me^4}{2\hbar^3 c} \cdot \frac{\hbar^2}{me^2} = \frac{e^2}{2\hbar c} = \frac{\alpha}{2} \ll 1$$

- Another approximation we made was to neglect coupling of light B-field with electron's magnetic moment μ. Including this, we have for the –

- Coulomb-gauge Hamiltonian:

$$H_1 = \frac{e}{mc}\mathbf{p}\cdot\mathbf{A} - \mu\cdot\mathbf{B}$$

Multipole transitions for Segway™ riders

- Expanding the exponent:

$$e^{i\mathbf{k}\cdot\mathbf{r}} = 1 + i(\mathbf{k}\cdot\mathbf{r}) - \frac{(\mathbf{k}\cdot\mathbf{r})^2}{2} + \ \ldots$$

- It is possible to build a classification of multipole transitions based on this expansion, for example, E2 first appears in the second term
- However, complications: magnetic multipoles, etc.
- Nice way to sort this out: photon picture: $j = l, l+1, \text{or} l-1$
  - Multipolarity determined by *j* :

$$\text{dipole for } j = 1, \text{ quadrupole for } j = 2, \text{ octupole for } j = 3, \text{ etc.}$$

  - E or M ? $\Rightarrow$ $j = l \pm 1 \text{ (electric)}, \text{ or } j = l \text{ (magnetic)}$

Multipole transitions for Segway™ riders
connecting the photon and semiclassical pictures

- The Rayleigh's formula:

$$e^{i\mathbf{k}\cdot\mathbf{r}} = \sum_{l=0}^{\infty} i^l (2l+1) j_l(kr) P_l(\cos\theta)$$

Spherical Bessel Functions

Legendre Polynomials

- Property of Bessel functions: expanding $j_l(kr)$

  we get nonzero terms with $(kr)^l, (kr)^{l+2}, (kr)^{l+4}, \text{ etc.}$

Multipole transitions for Segway™ riders
some examples

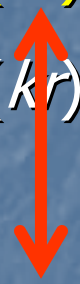
- E1: j=1 (dipole); l=0 (the only way with $j=l\pm1$)

  For l=0, nonzero terms in the Rayleigh's formula are 1, $(kr)^2$, …
- E2: j=2 (qadr.); l=1 or 3 (because $j=l\pm1$)

  For l=1, nonzero terms in Rayleigh's formula are (kr), $(kr)^3$, …

  For l=3, nonzero terms in Rayleigh's formula are $(kr)^3$, $(kr)^5$, …
- M1: j=1 (dipole); l=1 (because $j=l$)

  For l=1, nonzero terms in Rayleigh's formula are (kr), $(kr)^3$, …
- The photon picture is consistent with semiclassical one



Multipole transitions for Segway™ riders

photon quantum numbers and selection rules

Multipole	E1	M1	E2	M2	E3
Power of kr	0,2,...	1,3,...	1,3,...	2,4,...	2,4,...
photon l	0	1	1,3	2	2,4
photon j	1	1	2	2	3
atom ΔJ	$\pm 1, 0$	$\pm 1, 0$	$\pm 2, \pm 1, 0$	$\pm 2, \pm 1, 0$	$\pm 3, \pm 2, \pm 1, 0$
	$0 \nleftrightarrow 0$	$0 \nleftrightarrow 0$	$0 \nleftrightarrow 0, 1$	$0 \nleftrightarrow 0, 1$	$0 \nleftrightarrow 0, 1, 2; 1 \nleftrightarrow 1$
photon parity $(-1)^{l+1}$	-1	1	1	-1	-1
atom parity change	yes	no	no	yes	yes

D. DeMille, D. Budker, N. Derr, and E. Deveney, How we know that photons are bosons: experimental tests of spin-statistics for photons, in: Proceedings of the International Conference on Spin-Statistics Connection and Commutation Relations: Experimental Tests and Theoretical Implications, Anacapri, Italy, May 31-June 3, 2000, R. C. Hilborn and G. M. Tino, Eds., AIP Conf. Procs. #545, 2000, p. 227.

Multipole transitions for Segway™ riders

A generic estimate of relative transition intensities

- Consider an electron or nucleon of charge *e* and mass *m* localized in a system (atom, nucleus, …) of characteristic dimensions *R*
- A crude estimate of allowed Eκ and Mκ matrix elements :

$$M.E.(\mathrm{E}\kappa) \sim eR^{\kappa},$$

$$M.E.(\mathrm{M}\kappa) \sim \frac{e\hbar}{2mc} R^{\kappa-1}$$

- Next, we wish to generalize the result for spontaneous decay rate we discussed earlier :

$$\left|(\xi' J' \| d \| \xi J)\right|^2 \frac{1}{2J'+1} \frac{4\omega_0^3}{3\hbar c^3} = \frac{1}{\tau}$$

Multipole transitions for Segway™ riders

A generic estimate of relative transition intensities

- Spontaneous decay rate is $\propto |\text{M.E.}|^2(k)^{\text{appropr.power}}\left(\omega^3/(\hbar c^3)\right)$

$$M.E.(\mathrm{E}\kappa) \sim eR^{\kappa},$$

$$M.E.(\mathrm{M}\kappa) \sim \frac{e\hbar}{2mc} R^{\kappa-1}$$

- Which results in :

$$\Gamma(\mathrm{E}\kappa) \sim e^2 R^{2\kappa} \frac{k^{2\kappa+1}}{\hbar},$$

$$\Gamma(\mathrm{M}\kappa) \sim \left(\frac{e\hbar}{2mc}\right)^2 R^{2\kappa-2} \frac{k^{2\kappa+1}}{\hbar}$$

$$\left|(\xi' J' \| d \| \xi J)\right|^2 \frac{1}{2J'+1} \frac{4\omega_0^3}{3\hbar c^3} = \frac{1}{\tau}$$

Multipole transitions for Segway™ riders

A generic estimate of relative transition intensities

- In atoms, for transitions of comparable frequency,

$$\frac{\Gamma(\mathrm{E}\kappa)}{\Gamma(\mathrm{E1})} \sim (ka_0)^{2\kappa-2} \sim \left(\frac{\alpha}{2}\right)^{2\kappa-2},$$

$$\frac{\Gamma(\mathrm{M}\kappa)}{\Gamma(\mathrm{E1})} \sim \left(\frac{\hbar}{2a_0 mc}\right)^2 (ka_0)^{2\kappa-2} \sim \left(\frac{\alpha}{2}\right)^{2\kappa}$$

- Note different $k(\omega)$ dependences for different multipoles

Example: γ-ray emission by nuclei

- In light nuclei, typical γ-ray energy is ~ MeV :

$$k = \frac{\omega}{c} = \frac{\hbar\omega}{\hbar c} \sim \frac{1\ \mathrm{MeV}}{197\ \mathrm{MeV}\cdot\mathrm{fm}}$$

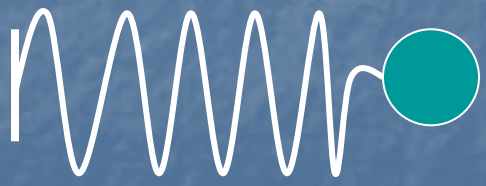
- while nuclear size R is on the order of a few fermi

(1 fermi = 1 fm = 10^{-13} cm)

- Ratio between system size and wavelength similar to that for atoms
- However, high-multipolarity transitions are often important; this is when low-multipolarity transitions are suppressed by selection rules
  - High-angular-momentum excited states (nuclear isomers)
  - Isospin-symmetry suppression of many E1 transitions

Visualization of atomic transitions

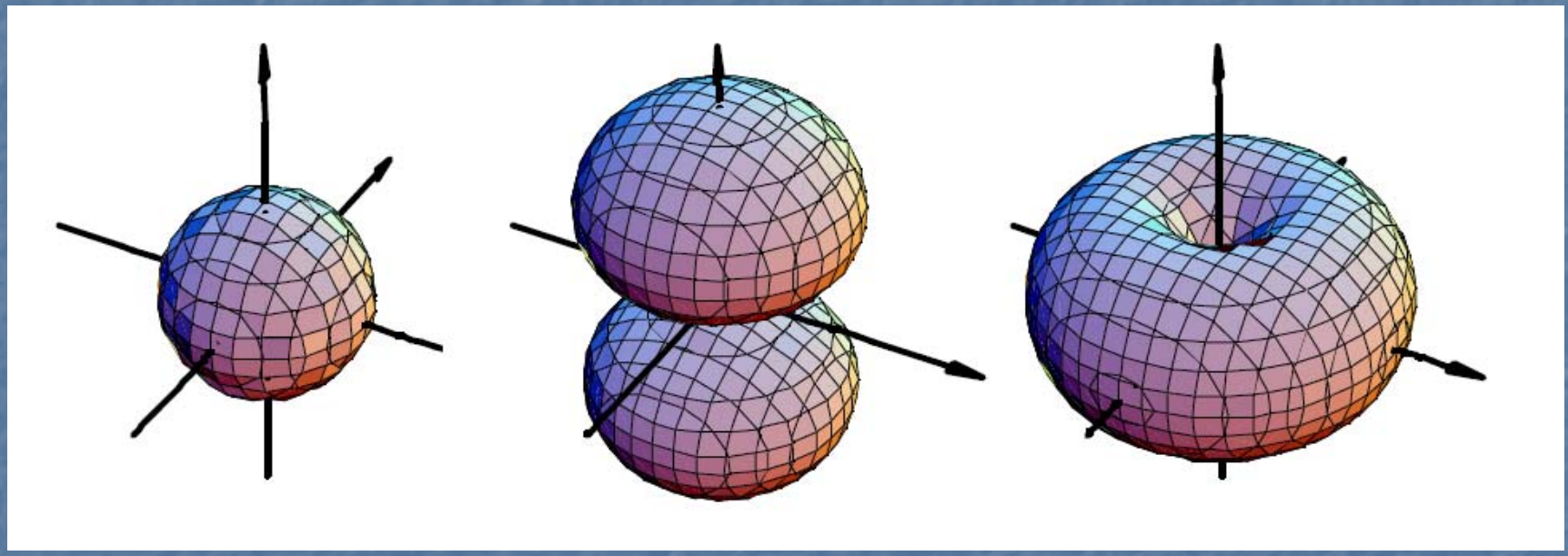
- In classical physics, linearly polarized radiation is associated with an oscillating linear dipole (electron on a spring)
- Circular or elliptical radiation are similarly associated with appropriately phased motion of the "electron on a spring" in two perpendicular directions
- Some physicists assert that all of atomic physics and the physics of light-atom interactions can be understood from the electron-on-a-spring picture
- We do not believe this to be quite true…
- In *some* cases, one needs **two** electrons on a spring !



Visualization of atomic transitions

- What about quantum physics ?
- An atom in an energy eigenstate has NO dipole moment and cannot be associated with electron on a spring

Electron-density plots (hydrogen)



1S 2P (M=0) 2P (M=±1)

- Symmetric charge distr. ⇒ no electric dipole ⇒ no radiation !

Visualization of atomic transitions

- Q: Where does the dipole originate ?
- A: From superpositions of energy eigenstates
- Consider a specific transition $|2P, M' = 0\rangle \rightarrow |1S, M = 0\rangle$
- Let us examine a coherent superposition of these two states:

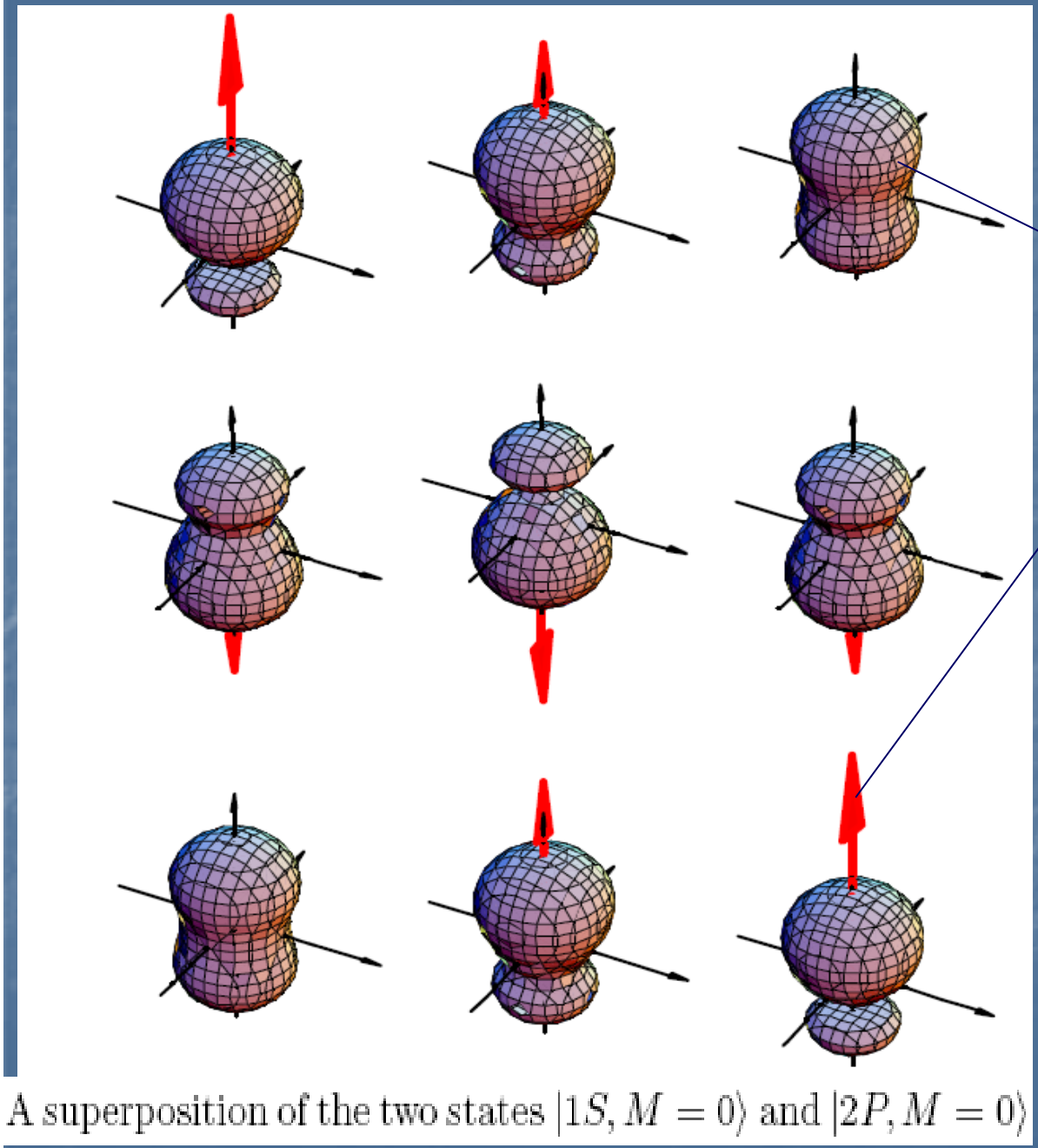
$$a|1S, M = 0\rangle + e^{-iE_2 t/\hbar} a' |2P, M' = 0\rangle$$

- with the usual demand that $|a|^2 + |a'|^2 = 1$
- Pick a particular situation

$$a = a' = \frac{1}{\sqrt{2}}.$$

- Bingo !

Visualization of atomic E1 transitions



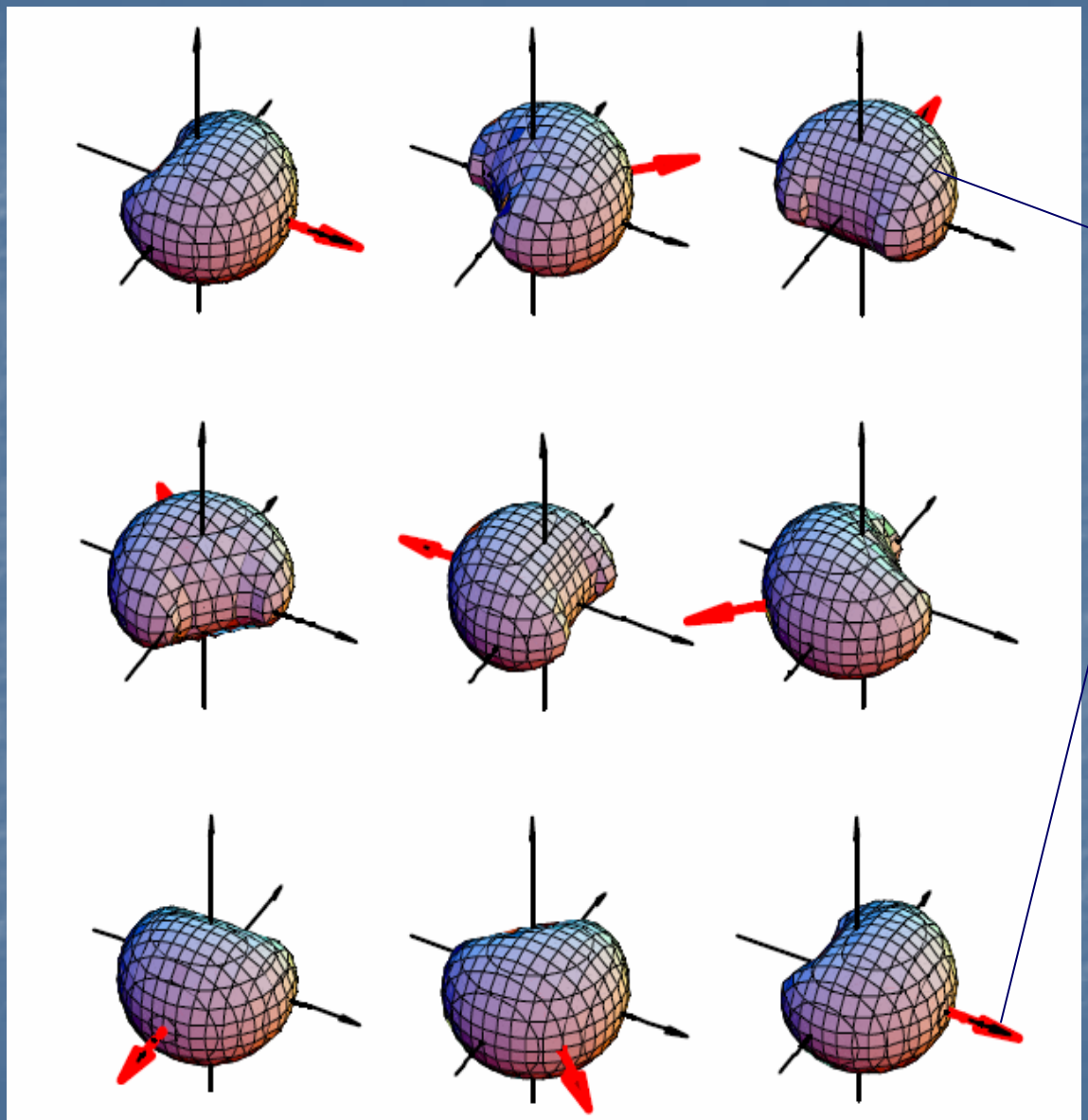
A superposition of the two states $|1S, M = 0\rangle$ and $|2P, M = 0\rangle$

Instantaneous electron density

Instantaneous dipole moment

Corresponds precisely to dipole moment oscillating along z and emitting **linearly polarized** light !

Visualization of atomic E1 transitions



A superposition of the two states $|1S, M = 0\rangle$ and $|2P, M = 1\rangle$

Instantaneous electron density

Instantaneous dipole moment

Corresponds precisely to dipole moment rotating around z and emitting **circularly polarized** light !

Visualization of atomic E1 transitions

- An important issue: if the atom is initially in the $2P$ state, how does the initial mixing with $1S$ occur ?
- The agent is spontaneous emission, to which there is

NO CLASSICAL ANALOGY !

- Spontaneous Emission – due to vacuum fluctuations of E/M field

"Spontaneous Emission" in concert, Berkeley, Dec. 2003

- Similar treatment for absorption (but only stimulated)

Visualization of atomic M1 transitions

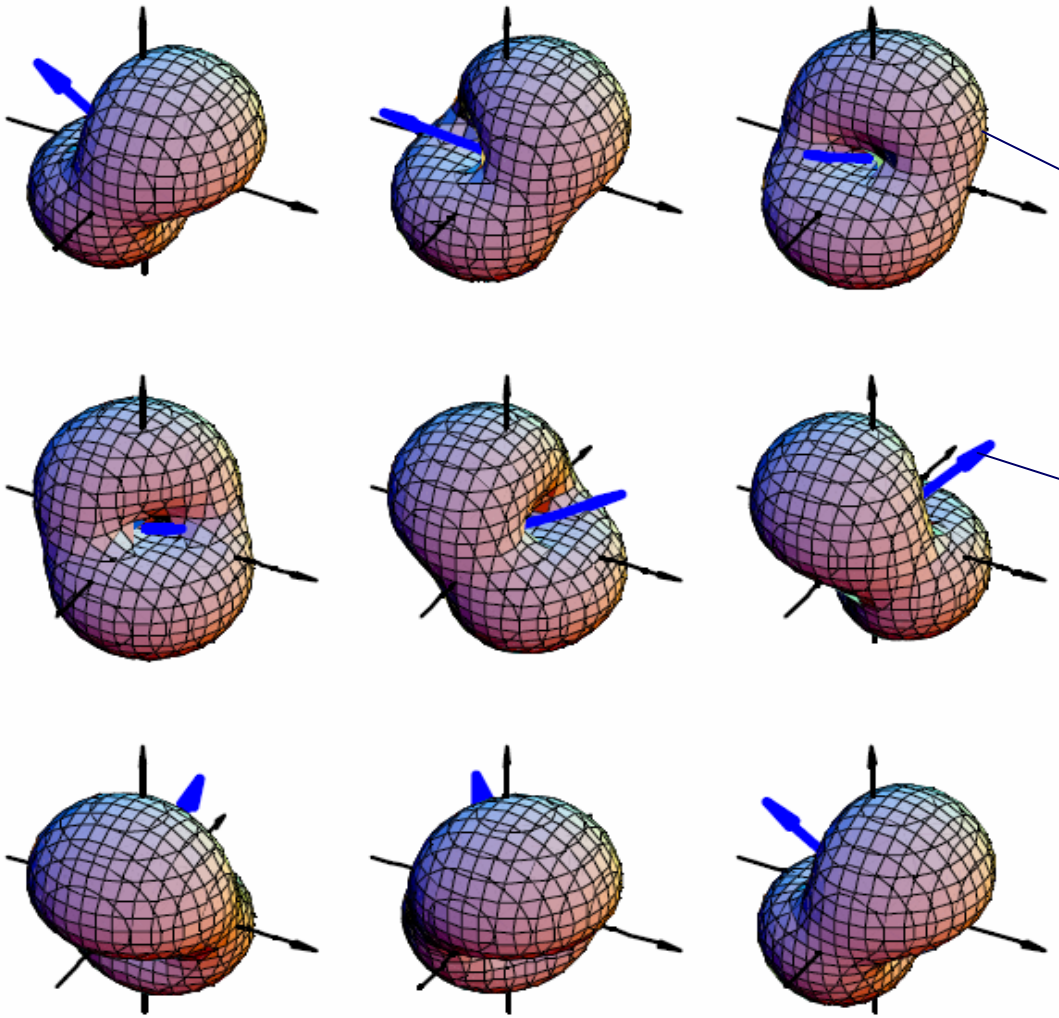


Figure 5.9: Electron density for a coherent superposition of the $|2P, M = 0\rangle$ and $|2PM = 1\rangle$ states. The nonzero value of energy splitting between these states can result, for example, from Zeeman shift of the $M = 1$ magnetic sublevel. One period of Larmor precession is shown. The arrow indicates the instantaneous direction and magnitude of the magnetic-dipole moment.

Instantaneous electron density (no electric-dipole)

Instantaneous magnetic dipole moment

$$\mu = \frac{1}{2c}\int \mathrm{r} \times \mathrm{j}(\mathrm{r}) d^3 r$$

Corresponds precisely to magnetic moment rotating around **B** and emitting **circularly polarized** rf radiation !