J Matrices

Last time:

starting with $\left[\mathbf{J}_i, \mathbf{J}_j\right] = i\hbar \sum_k \varepsilon_{ijk} \mathbf{J}_k$ DEFINITION !

$$\mathbf{J}^2 |jm\rangle = \hbar^2 j(j+1) |jm\rangle$$

$$\mathbf{J}_z |jm\rangle = \hbar m |jm\rangle$$

$$\mathbf{J}_\pm = \mathbf{J}_x \pm i\mathbf{J}_y$$

$$\mathbf{J}_\pm |jm\rangle = \hbar\left[j(j+1) - m(m\pm 1)\right]^{1/2} |jm\pm 1\rangle$$

nonzero matrix elements and “Condon Shortley” phase choice

$$\langle j'm'|\mathbf{J}^2|jm\rangle = \hbar^2 j(j+1)\delta_{j'j}\delta_{m'm}$$

$$\langle j'm'|\mathbf{J}_z|jm\rangle = \hbar m\delta_{j'j}\delta_{m'm}$$

$$\langle j'm'|\mathbf{J}_\pm|jm\rangle = \hbar\left[j(j+1) - mm'\right]^{1/2}\delta_{j'j}\delta_{m'm\pm 1}$$

$\left(\mathbf{J}^2, \mathbf{J}_z, \mathbf{J}_x, \mathbf{J}_y, \mathbf{J}_+, \mathbf{J}_-\right)$ all stay within j

all matrix elements of $\mathbf{J}^2, \mathbf{J}_z, \mathbf{J}_x, \mathbf{J}_\pm$ are real and positive (only those of $\mathbf{J}_y$ are imaginary)

TODAY:
1. What do the matrices look like for $J = 0,\ 1/2,\ 1$?
2. many operators are expressed as an angular momentum times a constant — Zeeman example — density matrix
3. other operators involve things like $\vec{q}$ or products of two angular momenta

Stark effect

Wigner-Eckart Theorem

* classify operators by commutation rule
* matrix elements in convenient basis sets
* transform between inconvenient and convenient basis sets.

$\left[\mathbf{p}_x, \mathbf{p}_y\right] = 0$

A student in 1999 suggested that he could find *f(x,y)* such that

$$\frac{\partial^2 f}{\partial x \partial y} \neq \frac{\partial^2 f}{\partial y \partial x} \qquad \text{Thus } \left[\mathbf{p}_x, \mathbf{p}_y\right] \neq 0!$$

This is possible, but *f(x,y)* would have to have a form that excludes it as an acceptable $\psi(x,y)$. Typically, the *f(x,y)* will have to be discontinuous or have discontinuous first derivatives. For all well behaved *V(x,y)*, $\psi(x,y)$ will have continuous first derivatives. The *f(x,y)* used to prove a commutation rule must be acceptable as a quantum mechanical wavefunction, $\psi(x,y)$. This is a good thing because (see Angular Momentum Handout)

$$e^{-ia\mathbf{p}_x/\hbar}\left|x_1\right\rangle = \left|x_1 + a\right\rangle$$

$e^{-ia\mathbf{p}_x/\hbar}$ generates a linear translation of $+a$ in x direction.

linear translations commute (but rotations do not)

This is the basis for (or a consequence of) $\left[\mathbf{p}_i, \mathbf{p}_j\right] = 0$

$$\left[\mathbf{J}_i, \mathbf{J}_j\right] = i\hbar \sum_k \varepsilon_{ijk} \mathbf{J}_k$$

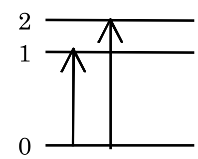
Nonlecture

prepare (excite) $\mathbf{E}$
evolve $e^{-i\mathbf{H}t/\hbar}$
detect $\mathbf{D}$

e.g. basis set $|0\rangle, |1\rangle, |2\rangle$

excite:
$$\mathbf{E}|0\rangle = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$$

The "excitation matrix" $\mathbf{E}$ creates equal amplitudes in two excited eigenstates:



$$\boldsymbol{\rho}(0) = \mathbf{E}|0\rangle\langle 0|\mathbf{E}^\dagger$$

evolve: If we are in the eigenbasis of $\mathbf{H}$
$$e^{-iHt/\hbar}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} ae^{-iE_a t/\hbar} \\ be^{-iE_b t/\hbar} \\ ce^{-iE_c t/\hbar} \end{pmatrix}$$
(translation in time)

but otherwise, need $\left[\mathbf{T}e^{-i\mathbf{T}^\dagger\mathbf{H}\mathbf{T}t/\hbar}\mathbf{T}^\dagger\right] = \mathbf{U}(t,0)$

$$\begin{aligned}\boldsymbol{\rho}(t) &= \mathbf{T}e^{-i\mathbf{T}^\dagger\mathbf{H}\mathbf{T}\,t/\hbar}\underbrace{\mathbf{T}^\dagger\mathbf{E}|0\rangle\langle 0|\mathbf{E}^\dagger\mathbf{T}}_{\boldsymbol{\rho}(0)\text{ in eigenbasis of }\mathbf{H}}e^{+i\mathbf{T}^\dagger\mathbf{H}\mathbf{T}\,t/\hbar}\mathbf{T}^\dagger \\ &= \mathbf{U}(t,0)\boldsymbol{\rho}(0)\mathbf{U}^\dagger(t,0)\end{aligned}$$

detect: $\mathbf{D}$ the "detection matrix"

$$\langle\mathbf{D}\rangle_t = \text{Trace}(\boldsymbol{\rho}\mathbf{D})$$

Building Blocks

Many QM operators have the form $f(\vec{\mathbf{J}})$

e.g. Zeeman effect $\mathbf{H}^{\text{Zeeman}} = -\gamma\vec{B}\cdot\mathbf{J}$ ($\vec{B}$ is magnetic field)

Others have the form $f(\vec{\mathbf{q}})$

e.g. Stark effect $\mathbf{H}^{\text{Stark}} = e\vec{E}\cdot\vec{\mathbf{q}}$ ($\vec{E}$ is electric field)

[Others have the form of $f(\mathbf{J}_1,\mathbf{J}_2)$

e.g. spin - orbit $\mathbf{H}^{SO} = a\mathbf{L}\cdot\mathbf{S}$

We are going to want to be able to write matrix representations of these operators.

Let us begin by writing matrices for $\mathbf{J}^2$, $\mathbf{J}_z$, $\mathbf{J}_x$, $\mathbf{J}_y$, $\mathbf{J}_+$, $\mathbf{J}_-$.

$\boxed{j = 0}$ only basis state is $|jm\rangle = |00\rangle$
1 × 1 matrix

$$\mathbf{J}^2|00\rangle = \begin{pmatrix} 0 \end{pmatrix}$$

same for all components

$\boxed{j = 1/2}$ $\left|\frac{1}{2}\frac{1}{2}\right\rangle$ and $\left|\frac{1}{2}-\frac{1}{2}\right\rangle$ 2×2 matrices

$$\mathbf{J}^{2(1/2)} = \frac{3}{4}\hbar^2\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} \qquad \mathbf{J}^2\left|\frac{1}{2}\frac{1}{2}\right\rangle = \hbar^2\frac{1}{2}\left(\frac{1}{2}+1\right)\left|\frac{1}{2}\frac{1}{2}\right\rangle$$

$$\mathbf{J}_z^{(1/2)} = \frac{1}{2}\hbar\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \qquad \text{e.g.} \quad \begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix}\underbrace{\begin{pmatrix}1\\ 0\end{pmatrix}}_{\boxed{m=+1/2}} = \begin{pmatrix}0\\ 0\end{pmatrix} \qquad \mathbf{J}_+^{(1/2)}\left|\frac{1}{2}\frac{1}{2}\right\rangle = 0$$

$$\mathbf{J}_+^{(1/2)} = \hbar\begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix} \qquad \begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix}\underbrace{\begin{pmatrix}0\\ 1\end{pmatrix}}_{\boxed{m=-1/2}} = \begin{pmatrix}1\\ 0\end{pmatrix} \qquad \mathbf{J}_+^{(1/2)}\left|\frac{1}{2}-\frac{1}{2}\right\rangle = \hbar\left|\frac{1}{2}\frac{1}{2}\right\rangle$$

$$\mathbf{J}_{-}^{(1/2)} = \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

$$\mathbf{J}_{x}^{(1/2)} = \frac{1}{2}(\mathbf{J}_{+} + \mathbf{J}_{-}) = \frac{1}{2}\hbar\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\mathbf{J}_{y}^{(1/2)} = \frac{1}{2i}(\mathbf{J}_{+} - \mathbf{J}_{-}) = -\frac{i}{2}\hbar\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

verify that $\boldsymbol{J}^2 = \boldsymbol{J}_x^2 + \boldsymbol{J}_y^2 + \boldsymbol{J}_z^2$

$$\left(\mathbf{J}^{(1/2)}\right)^2 = \frac{3\hbar^2}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\mathbf{J}_x^2 = \frac{\hbar^2}{4}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{\hbar^2}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\mathbf{J}_y^2 = \frac{\hbar^2}{4}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \frac{\hbar^2}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

An amazing amount of insight gained from this complete set of 2×2 matrices

$$\mathbf{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\left[\begin{array}{l} \boldsymbol{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \rightarrow \mathbf{J}_x^{(1/2)} \\ \boldsymbol{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \rightarrow \mathbf{J}_y^{(1/2)} \\ \boldsymbol{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \rightarrow \mathbf{J}_z^{(1/2)} \end{array}\right.$$

3 matrices with eigenvalues ± 1

CTDL, pages 417-454
1. Pauli Matrices
2. Diagonalization of 2×2
3. Geometric interpretation of 2×2 $\boldsymbol{\rho}$ in terms of fictitious spin 1/2
4. spin 1/2 $\boldsymbol{\rho}$
5. magnetic resonance

What is $[\boldsymbol{\sigma}_x, \boldsymbol{\sigma}_y] = ?$

arbitrary $\mathbf{M} = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} = \frac{m_{11}+m_{22}}{2}\mathbf{I} + \frac{m_{11}-m_{22}}{2}\boldsymbol{\sigma}_z + \frac{m_{12}+m_{21}}{2}\boldsymbol{\sigma}_x + i\frac{m_{12}-m_{21}}{2}\boldsymbol{\sigma}_y$

$$\mathbf{M} = \underbrace{a_0}_{\boxed{\text{scalar part of } \mathbf{M}}}\mathbf{I} + \underbrace{\vec{a}}_{\boxed{\text{vector part of } \mathbf{M}}} \cdot \vec{\sigma}$$

$a_0 = \frac{1}{2}Tr(\mathbf{M})$ Center of Gravity

$\vec{a} = \frac{1}{2}Tr(\mathbf{M}\boldsymbol{\sigma})$ $\mathbf{M} \leftrightarrow \boldsymbol{\rho}$

$$\boxed{\begin{aligned} a_x &= \frac{1}{2}\mathrm{Tr}(\mathbf{M}\boldsymbol{\sigma}_x) \\ a_y &= \frac{1}{2}\mathrm{Tr}(\mathbf{M}\boldsymbol{\sigma}_y) \\ a_z &= \frac{1}{2}\mathrm{Tr}(\mathbf{M}\boldsymbol{\sigma}_z) \end{aligned}}$$

Information in $2 \leftrightarrow 2$ $\boldsymbol{\rho}$ is repackaged into a 3 component vector. Visualization of dynamics!

This provides a basis for taking apart the dynamics of an arbitrary 2×2 $\boldsymbol{\rho}$ into dynamics of *x, y, z* fictitious spin-1/2 components. Beat the $S = 1/2$ Zeeman problem to death and use it as basis for understanding dynamics of any 2×2 space.

J = 1 A set of 3 × 3 matrices

$$\mathbf{J}^{2^{(1)}} = 2\hbar^2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\mathbf{J}_z^{(1)} = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$\mathbf{J}_+^{(1)} = 2^{1/2}\hbar \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

$$\mathbf{J}_+^{(1)}|11\rangle = 0$$

$$\mathbf{J}_-^{(1)} = 2^{1/2}\hbar \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

$$\mathbf{J}_x^{(1)} = 2^{-1/2}\hbar \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

$$\mathbf{J}_y^{(1)} = 2^{-1/2}\hbar \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$

For 2 × 2 problem (e.g. J = 1/2), needed 4 independent 2 × 2 matrices (because there are 4 elements in a 2 × 2 matrix) to represent arbitrary 2 × 2 matrix.

for 3 × 3 problem, need 9 independent 3 × 3 matrices

$\left(\mathrm{x,y,z,\ \ x^2,y^2,z^2,\ \ xy,xz,yz}\right)$ (because there are 9 elements in a 3 × 3 matrix)

actually scalar (I), vector, tensor

$\mathrm{s + p + d}$

[for 2 × 2 it was $s + p = 4$].

Can you write out each of the $\mathrm{J}^{(3/2)}$ matrices (16 4 ↔4 matrices)?

9 3×3 basis matrices is not nearly so nice as the 4 basis matrices for 2×2 problem. But this turns out to be what is needed to "understand" and picture spin = 1 systems.

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similarly for $j = 3/2,\ 2$, etc.

There are 2 lovely consequences of being able to take an arbitrary matrix and rewrite it as sum of **J** matrices.

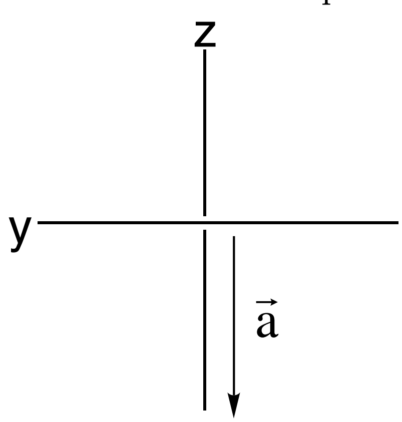
1. If **M** is the matrix of an operator – a term in the Hamiltonian – then it is clear that this operator may be re-expressed as a sum of operators, each of which behaves exactly like a (combination of) component(s) of **J** – evaluated in the $|jm\rangle$ basis set.

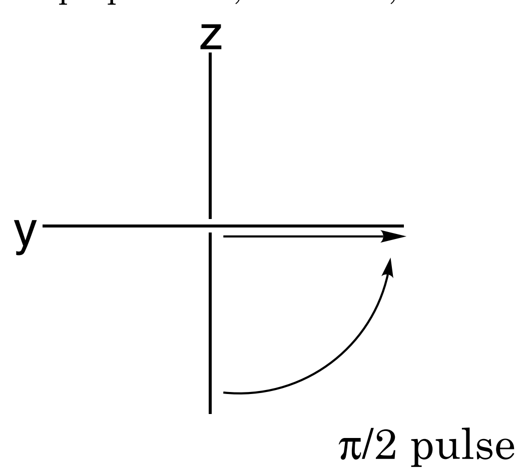
$$\mathbf{M}^{(j)} = a_0\mathbf{I} + \sum_i a_{li}\mathbf{J}_i\mathbf{J}_j + \sum_{i,j,k} c_{3ijk}\mathbf{J}_i\mathbf{J}_j\mathbf{J}_k + \ldots$$

   basis for classification of operators into $T_m^{(k)}$

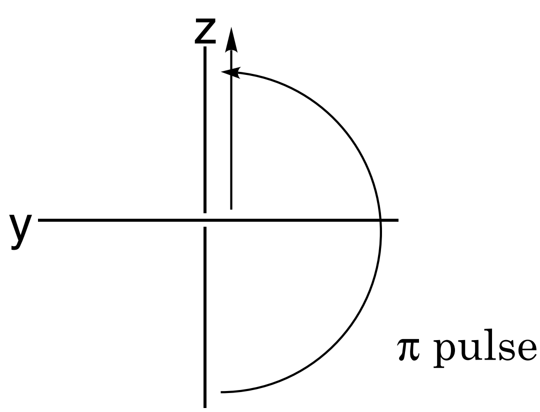
   and Wigner– Eckart Theorem for evaluation of matrix elements.

2. especially for 2 level systems, if $\mathbf{M} = \boldsymbol{\rho}$ and $\vec{a}$ is defined from **M** as on page 24-6, then we have a vector picture to understand preparation, evolution, detection



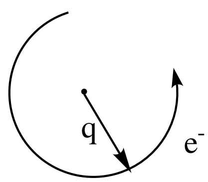


evolution of vector, fictitious B-fields



Now let's do some J = 1 examples

Zeeman effect for an $\ell = 1$, (p orbital) state



current on a circular wire

$$\vec{\mathbf{L}} = \vec{\mathbf{q}} \times \vec{\mathbf{p}} \qquad \text{(up out of page)}$$
$$\vec{\boldsymbol{\mu}}_L \propto -\vec{\mathbf{q}} \times \vec{\mathbf{p}} \qquad \text{(down into page)}$$
$$\vec{\boldsymbol{\mu}}_L \propto -\vec{\mathbf{L}} \qquad \vec{\boldsymbol{\mu}}_L \equiv -\gamma\vec{\mathbf{L}}$$

classical energy $\quad E = \overset{\boxed{\text{field strength}}}{\vec{B}} \cdot \boldsymbol{\mu}_L = \underbrace{B_z}_{\boxed{\text{field exclusively along z}}}\hat{k} \cdot \left(-\gamma\vec{\mathbf{L}}\right) = -\gamma B_z \mathbf{L}_z$

for $L = 1$ system: $\quad \mathbf{H}^{Zeeman} = -\gamma B_z \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$

<u>case (1)</u> Let $\Psi(0) = |LM_L\rangle = |11\rangle$

$$\boldsymbol{\rho} = |\Psi\rangle\langle\Psi| = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$E_{LM_L} = E_{11} = Trace(\boldsymbol{\rho}\mathbf{H})$$
$$= -\hbar\gamma B_z Tr\left[\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}\right]$$
$$= -\hbar\gamma B_z$$

$$\boldsymbol{\rho} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

What about? $E_{10} = \text{Trace }(\boldsymbol{\rho}\mathbf{H}) = \mathbf{0}$

$E_{1-1} = +\gamma B_z \hbar$ no motion of E

<u>case (2)</u> Let $\Psi(0) = 2^{-1/2}\left(|11\rangle + |10\rangle\right)$

$$\Psi(t) = 2^{-1/2}\left[|11\rangle e^{-iE_{11}t/\hbar} + |10\rangle e^{-i0t/\hbar}\right]$$

$$\boldsymbol{\rho}(t) = \frac{1}{2}\left(|11\rangle\langle 11| + |10\rangle\langle 10| + |11\rangle\langle 10| e^{-iE_{11}t/\hbar} + |10\rangle\langle 11| e^{+iE_{11}t/\hbar}\right)$$

$$\boldsymbol{\rho}(t) = \frac{1}{2}\begin{pmatrix} 1 & e^{-i\omega_{11}t} & 0 \\ e^{i\omega_{11}t} & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

nothing at location of coherence in $\boldsymbol{\rho}$

$$\mathbf{H}(B \parallel +z) = -\gamma B_z \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$E(t) = \langle \mathbf{H} \rangle = \text{Trace}(\mathbf{H}\boldsymbol{\rho}) = -\frac{1}{2}\gamma B_z \hbar (1)$$ no motion of E

Looked at 2 cases:

1. pure state $|11\rangle, B \parallel z$ $\quad E = -\gamma B_z \hbar$
2. mixed state $2^{-1/2}\left(|11\rangle + \langle 10|\right), B \parallel z$

$$E = -\frac{1}{2}\gamma B_z \hbar$$

always mixed state gives time independent $\langle E \rangle$

NMR: oscillating B_x, B_y, cw B_z

Stark Effect: Electric field

classical $E \propto \vec{\varepsilon} \cdot \left(\vec{q}_{e^-} - \vec{q}_{p^+}\right) \approx \varepsilon_z \boldsymbol{z}$

so we will need matrix elements of $\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z}$ in $|\mathrm{jm}\rangle$ basis set. How?

Based on $\left[z, \boldsymbol{L}_j\right] = -i\hbar \sum_k \varepsilon_{zjk} \boldsymbol{q}_k$ vector operator definition — later

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Other angular momenta

1. $\boldsymbol{\ell}$ electron orbital ang. mom.
2. $\mathbf{s}$ electron spin
3. $\mathbf{I}$ nuclear spin

These separate angular momenta interact with each other

spin - orbit: $\boldsymbol{\zeta}(\mathrm{r}) \boldsymbol{\lambda} \cdot \mathbf{s}$

Zeeman: $-\gamma \mathrm{B}_{\mathrm{z}}\left(\mathbf{L}_{\mathrm{z}} + \mathrm{g}_{\mathrm{s}} \mathbf{S}_{\mathrm{z}} + \mathrm{g}_{\mathrm{I}} \mathrm{I}_{\mathrm{z}}\right)$

hyperfine: $\mathrm{a}\, \mathrm{I} \bullet \mathrm{S}$

coupled and uncoupled basis sets: $|\ell m_\ell\rangle |s m_s\rangle \leftrightarrow |j \ell s m_j\rangle$

<u>case (3)</u>

$$\text{same } \Psi(0) = 2^{-1/2}(|11\rangle + |10\rangle)$$

but $\mathbf{H}$ is for $\vec{B} \parallel x$

one at coherence in $\boldsymbol{\rho}$

$$\mathbf{H} = -\gamma B_x \hbar 2^{-1/2} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

Something subtle is intentionally wrong here. Can you find it?

$$E(t) = Tr(\mathbf{H}\boldsymbol{\rho}) = -\frac{1}{2}\gamma B_x \hbar\left[e^{+i\omega_{11}t} + e^{-i\omega_{11}t} + 0\right]$$
$$= -\gamma B_x \hbar \cos \omega_{11} t$$