

J Matrices

Last time:

starting with $[J_i, J_j] = i\hbar \sum_k \epsilon_{ijk} J_k$

DEFINITION OF AN ANGULAR MOMENTUM !

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

$$J_z |jm\rangle = \hbar m |jm\rangle$$

$$J_{\pm} = J_x \pm iJ_y$$

$$J_{\pm} |jm\rangle = \hbar [j(j+1) - m(m \pm 1)]^{1/2} |jm \pm 1\rangle$$

nonzero matrix elements and “Condon Shortley” phase choice

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

$$\langle j'm' | J_z | jm \rangle = \hbar m \delta_{j'j} \delta_{m'm}$$

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

$(J^2, J_z, J_x, J_y, J_+, J_-)$ all stay within the same j quantum number

all matrix elements of J^2, J_z, J_x, J_y are real and positive (only those of J_{\pm} are imaginary)

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



Stark effect \uparrow

Wigner-Eckart Theorem

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

5.73 Lecture #24

24 - 2

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

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

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

This is possible, but $f(x,y)$ would have to have a form that excludes it as an acceptable $\Psi(x,y)$. Typically, such an $f(x,y)$ would 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 Lecture #22, page 22-7 or the Angular Momentum Handout)

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

$e^{-iap_x/\hbar}$ 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) $[\mathbf{p}_i, \mathbf{p}_j] = 0$

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

5.73 Lecture #24

Nonlecture

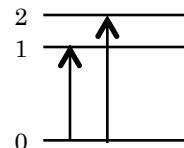
prepare (excite) **E**
 evolve $e^{-i\mathbf{H}t/\hbar}$
 detect **D**

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

This is artificial because it assumes that all population is moved from state 0 and transferred to states 1 and 2.

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”, **E**, creates equal amplitudes in two excited eigenstates:



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

evolve: If we are in the eigenbasis of **H**

$$e^{-i\mathbf{H}t/\hbar} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} ae^{-iE_a t/\hbar} \\ be^{-iE_b t/\hbar} \\ ce^{-iE_c t/\hbar} \end{pmatrix} \quad (\text{translation in time})$$

but if we are not in the eigenbasis of **H**, need $[\mathbf{T}e^{-i\mathbf{T}^\dagger\mathbf{H}\mathbf{T}t/\hbar}\mathbf{T}^\dagger] = \mathbf{U}(t,0)$

$$\rho(t) = \mathbf{T}e^{-i\mathbf{T}^\dagger\mathbf{H}\mathbf{T}t/\hbar}\mathbf{T}^\dagger\mathbf{E}|0\rangle\langle 0|\mathbf{E}^\dagger\mathbf{T}e^{+i\mathbf{T}^\dagger\mathbf{H}\mathbf{T}t/\hbar}\mathbf{T}^\dagger$$

$$= \mathbf{U}(t,0)\rho(0)\mathbf{U}^\dagger(t,0)$$

$\rho(0)$ in eigenbasis of **H**

This can be confusing because it is not clear what basis $\rho(0)$ is expressed in and what the appropriate **U** is for that basis set.

detect: **D** the “detection matrix”

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

Building Blocks!

5.73 Lecture #24

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

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

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

e.g. Stark effect $H^{\text{Stark}} = e\vec{\epsilon} \cdot \vec{q}$ ($\vec{\epsilon}$ 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 classes of operators. We are going to discover in this lecture that all of these operators have matrix representations that may be expressed as linear combinations of angular momentum matrices.

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 $|jm\rangle = |00\rangle$ $\frac{1}{2}(\mathbf{J}_x + i\mathbf{J}_y)$
 1×1 matrix

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

same for all components of \mathbf{J}

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

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

$$\mathbf{J}^2 \left| \frac{1}{2} \frac{1}{2} \right\rangle = \hbar^2 \frac{1}{2} \left(\frac{1}{2} + 1 \right) \left| \frac{1}{2} \frac{1}{2} \right\rangle$$

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

$$\mathbf{J}_+^{(1/2)} = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \xrightarrow{\text{e.g.}} \begin{matrix} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \\ \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{matrix} \quad \begin{matrix} \boxed{m = +1/2} \\ \boxed{m = -1/2} \end{matrix}$$

$$\mathbf{J}_+^{(1/2)} \left| \frac{1}{2} \frac{1}{2} \right\rangle = 0 \quad \mathbf{J}_+^{(1/2)} \left| \frac{1}{2} - \frac{1}{2} \right\rangle = \hbar \left| \frac{1}{2} \frac{1}{2} \right\rangle$$

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

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

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

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

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

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

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

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

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

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

3 matrices with eigenvalues ± 1

CTDL, pages 417-454

1. Pauli Matrices
2. Diagonalization of 2×2
3. Geometric interpretation of 2×2 ρ in terms of fictitious spin 1/2
4. spin 1/2 ρ
5. magnetic resonance

What is $[\sigma_x, \sigma_y] = ?$

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

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

$$([\sigma_x, \sigma_y]) = 2 \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} = 2i\sigma_z$$

Surprise? Why the 2?

$$\text{arbitrary } \mathbf{M} = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} = \frac{m_{11} + m_{22}}{2} \mathbf{I} + \frac{m_{11} - m_{22}}{2} \sigma_z + \frac{m_{12} + m_{21}}{2} \sigma_x + i \frac{m_{12} - m_{21}}{2} \sigma_y$$

$$\mathbf{M} = a_0 \mathbf{I} + \vec{a} \cdot \vec{\sigma}$$

scalar part of \mathbf{M}

vector part of \mathbf{M}

$$a_0 = \frac{1}{2} \text{Tr}(\mathbf{M})$$

Center of Gravity

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

$\mathbf{M} \leftrightarrow \rho$

$$a_x = \frac{1}{2} \text{Tr}(\mathbf{M}\sigma_x)$$

$$a_y = \frac{1}{2} \text{Tr}(\mathbf{M}\sigma_y)$$

$$a_z = \frac{1}{2} \text{Tr}(\mathbf{M}\sigma_z)$$

Information in 2×2 ρ is repackaged into a 3 component vector. Visualization of dynamics!

This provides a basis for taking apart the dynamics of an arbitrary 2×2 ρ 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 the dynamics in *any* 2×2 space.

5.73 Lecture #24

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We have done $J = 0$, $J = \frac{1}{2}$, now we do $J = 1$.

$J = 1$ A set of 3×3 matrices

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

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

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

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

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

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

An example:

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

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

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

For the 3×3 problem, we need 9 independent 3×3 matrices:

$(x, y, z, x^2, y^2, z^2, xy, xz, yz)$ (because there are 9 elements in a 3×3 matrix)

[actually one scalar (I), three vector, five second-rank tensor]

$$s + p + d = 9$$

[for 2×2 it was $s + p = 4$].

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

5.73 Lecture #24

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Nine 3×3 basis matrices for $\mathbf{J} = 1$ is not nearly as nice as the 4 basis matrices for the 2×2 $\mathbf{J} = 1/2$ problem. But this set of nine basis matrices turns out to be everything that is needed to “understand” and picture spin = 1 systems.

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

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

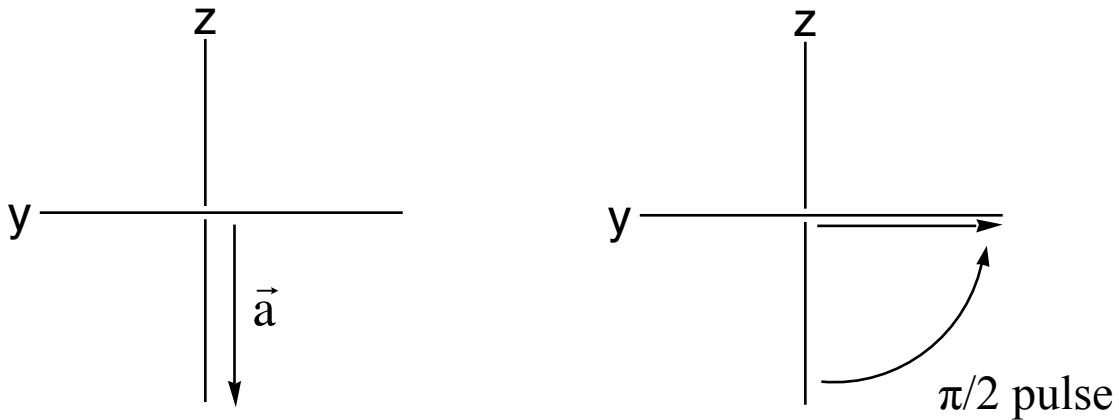
1. If \mathbf{M} is the matrix of an operator – a term in the Hamiltonian – then it is clear that this operator may be re-expressed as a sum of operators, each of which behaves exactly like a (combination of) component(s) of \mathbf{J} – evaluated in the $|jm\rangle$ basis set.

$$M^{(j)} = a_0 I + \sum_{i,j} (a_{1j} \mathbf{J}_i \mathbf{J}_j + \sum_{i,j,k} c_{3ijk} \mathbf{J}_i, \mathbf{J}_j, \mathbf{J}_k) + \dots$$

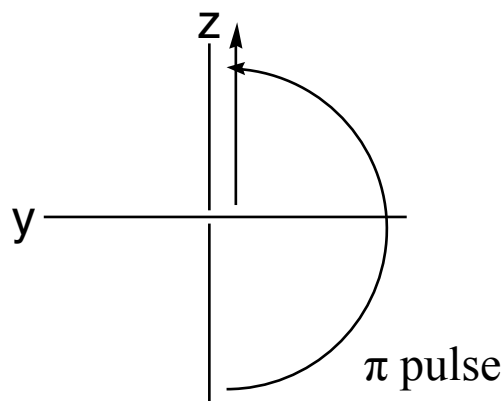
Cartesian vs. spherical tensor forms

This is the basis for classification of operators into $T_m^{(k)}$ (k -rank tensor, m -component) and the Wigner– Eckart Theorem for evaluation of matrix elements.

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

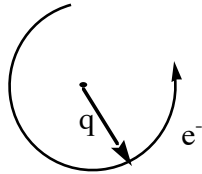


evolution of vector, fictitious B-fields



Now let's do some $J = 1$ examples

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



current on a circular wire

$$\begin{aligned} \vec{L} &= \vec{q} \times \vec{p} && \text{(up out of page)} \\ \vec{\mu}_L &\propto -\vec{q} \times \vec{p} && \text{(down into page)} \\ \vec{\mu}_L &\propto -\vec{L} && \vec{\mu}_L \equiv -\gamma \vec{L} \end{aligned}$$

right hand rule

field strength

classical energy

$$E = \vec{B} \cdot \vec{\mu}_L = B_z \hat{k} \cdot (-\gamma \vec{L}) = -\gamma B_z L_z$$

field exclusively along z

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

case (1) Let $\Psi(0) = |LM_L\rangle = |1 \ 1\rangle$

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

$$E_{LM_L} = E_{11} = \text{Trace}(\rho\mathbf{H})$$

$$\begin{aligned} &= -\hbar\gamma B_z \text{Tr} \left[\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \right] \\ &= -\hbar\gamma B_z \end{aligned}$$

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

What about?

$$E_{10} = \text{Trace}(\rho \mathbf{H}) = 0$$

$$E_{1-1} = +\gamma B_z \hbar$$

no motion of E

case (2): Let $\Psi(0) = 2^{-1/2} (|11\rangle + |10\rangle)$

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

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

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

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

zeroes at locations of coherence in ρ

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

Looked at 2 cases:

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

mixed state always gives time-independent $\langle E \rangle$ in \mathbf{H} is time-independent
 NMR: oscillating B_x, B_y , cw B_z . Many wonderful things happen!

Stark Effect: Electric field

classical $E \propto \vec{\epsilon} \cdot (\vec{q}_e - \vec{q}_{p^+}) \approx \epsilon_z z$

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

Based on $[z, L_j] = -i\hbar \sum_k \epsilon_{zjk} q_k$ from Vector operator definition (Lecture #23)
— later

Other angular momenta

1. ℓ electron orbital angular momentum
2. s electron spin
3. I nuclear spin

These separate angular momenta interact with each other

spin-orbit: $\zeta(r) \ell \cdot s$

Zeeman: $-\gamma B_z (\ell_z + g_s s_z + g_I I_z)$

hyperfine: $a \mathbf{I} \cdot \mathbf{s}$

We use coupled and uncoupled basis sets: $|\ell m_\ell\rangle |s m_s\rangle \leftrightarrow |j \ell s m_j\rangle$
to evaluate all matrix elements of these multiple-operator terms.

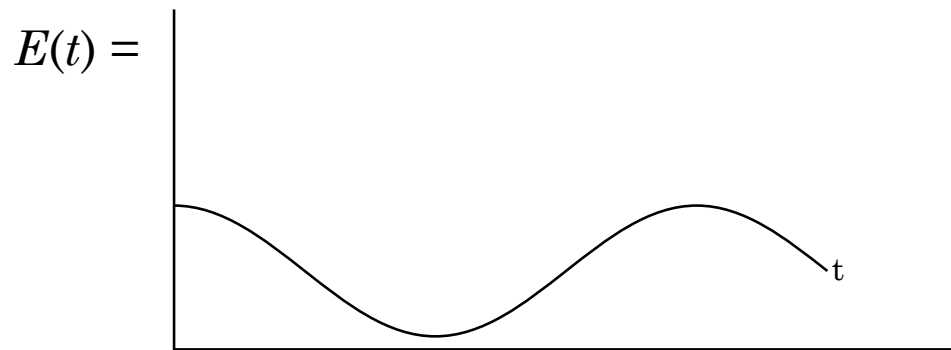
case (3): $\Psi(0) = 2^{-1/2} (|11\rangle + |10\rangle)$

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

$$\mathbf{H} = -\gamma B_x \hbar 2^{-1/2} \begin{pmatrix} 0 & \overset{\text{a one at the location of a coherence in } \rho}{1} & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

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

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



Put in t for t -dependent basis set, which is not the eigenbasis set.

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5.73 Quantum Mechanics I
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