Chapter 2

Dynamics of Two-Level Systems

In the last chapter we focused on eigenstate-based quantum mechanics. We will now be focusing on the dynamics of quantum systems that have two discrete energy levels, known as **two-level systems**. Before we introduce another formalism, let's attempt a simple example of two level systems. Now, let's attempt an example.

Problem 2.1: Potential Barrier

Consider two potential wells for an electron, well a and well b (these could, for example, be atomic nuclei). Each well binds an electron into a state with energy $E_a = E_b = E_0$ in the absence of the other well. When the two wells are brought close together there is a matrix element $\langle a | \hat{H} | b \rangle = t$ is real and increases as the distance between the wells decreases. **a.** Find the two solutions for the energy of the electron in terms of E_0 and t. **b.** If the two unperturbed wave functions are a and b, find the two solutions for the eigenfunctions and indicate which corresponds to which energy. **c.** Now apply an electric field to the system and approximate the effect of the electric field as changing E_a to $E_0 + \Delta$ and E_b to $E_0 - \Delta$. Find the energies and wave functions of the new eigenstates. **d.** How large must Δ/t be for one of the wave functions to be localised in well a with 90 percent probability?

Solution. First, we know that the Hamiltonian would be in the form,

$$\hat{H} = \hat{H}_{\text{original}} + \hat{H}_{\text{closeby}}.$$

In the basis $\{|a\rangle, |b\rangle\}$, we can express the Hamiltonian above as[1],

$$\hat{H} = \begin{pmatrix} E_0 & 0 \\ 0 & E_0 \end{pmatrix} + \begin{pmatrix} 0 & t \\ t & 0 \end{pmatrix} = \begin{pmatrix} E_0 & t \\ t & E_0 \end{pmatrix}$$

a/b. The first step here is to find the eigenvalues of the matrix representation of $\hat{H}$ in $\{|a\rangle, |b\rangle\}$ basis. Naturally, we can find the energy eigenvalues of this operator by computing the characteristic equation,

$$\hat{H} |\psi\rangle = E |\psi\rangle, \quad \rightarrow \quad \det \begin{pmatrix} E_0 - E & t \\ t & E_0 - E \end{pmatrix} = 0,$$

---

[1] Since t is real, we know that $\langle b | \hat{H} | a \rangle = \langle a | \hat{H} | b \rangle^\dagger = t^* = t$. Thus, the matrix elements of the "closeby" matrix would be $M_{ab} = M_{12} = M_{21} = t$.

which we can solve for E to be,

$$(E_0 - E)^2 - t^2 = 0, \quad \rightarrow \quad E_\pm = E_0 \pm t.$$

Now, we will try to find the eigenvectors corresponding to each eigenvalue. First, consider the eigenvalue $E_0 + t$. The eigenvector must obey the form,

$$\begin{pmatrix} E_0 & t \\ t & E_0 \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = (E_0 + t) \begin{pmatrix} A \\ B \end{pmatrix}.$$

Expanding the matrix multiplication, we find the system,

$$\begin{cases} AE_0 + Bt = A(E_0 + t) \\ At + BE_0 = B(E_0 + t) \end{cases}$$

It is clear that the tuple $A = 1, B = 1$ fulfils the system above. Normalising the system, we know that the first pair of eigenenergy/eigenstate would be,

$$\boxed{E_1 = E_0 + t, \quad |\psi_1\rangle = \frac{1}{\sqrt{2}}(|a\rangle + |b\rangle)}$$

Now, let's consider the second eigenenergy/eigenstate pair. Again, substituting the eigenenergy $E_0 - t$ into the eigensystem equation, we find,

$$\begin{pmatrix} E_0 & t \\ t & E_0 \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = (E_0 - t) \begin{pmatrix} A \\ B \end{pmatrix}, \quad \rightarrow \quad \begin{cases} AE_0 + Bt = A(E_0 - t) \\ At + BE_0 = B(E_0 - t) \end{cases}$$

Now, it is clear that the tuple $A = 1, B = -1$ satisfies the system above. Again, normalising the calculated eigenstate by dividing by $\sqrt{2}$, I find the second pair of eigenenergy/eigenstate to be,

$$\boxed{E_2 = E_0 - t, \quad |\psi_2\rangle = \frac{1}{\sqrt{2}}(|a\rangle - |b\rangle)}$$

c. The new Hamiltonian after replacing $E_a = E_0 + \Delta$ and $E_b = E_0 - \Delta$ would be,

$$\hat{H}_{\text{new}} = \begin{pmatrix} E_0 + \Delta & t \\ t & E_0 - \Delta \end{pmatrix}$$

Again, we can find the energy eigenvalues of this operator by computing the characteristic equation,

$$\hat{H} |\psi\rangle = E |\psi\rangle, \quad \rightarrow \quad \det \begin{pmatrix} E_0 + \Delta - E & t \\ t & E_0 - \Delta - E \end{pmatrix} = 0,$$

which we can solve to find,

$$(E_0 - E)^2 - \Delta^2 - t^2 = 0, \quad \rightarrow \quad E_\pm = E_0 \pm \sqrt{\Delta^2 + t^2}.$$

Again, we can find the eigenstate of this system by substituting the eigenenergy back into the eigenvalue problem and try to solve for the components of the eigenvector as follows.

$$\begin{pmatrix} E_0 + \Delta & t \\ t & E_0 - \Delta \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = (E_0 + \sqrt{\Delta^2 + t^2}) \begin{pmatrix} A \\ B \end{pmatrix}, \quad \rightarrow \quad \begin{cases} A(E_0 + \Delta) + Bt = A(E_0 + \sqrt{\Delta^2 + t^2}) \\ At + B(E_0 - \Delta) = B(E_0 + \sqrt{\Delta^2 + t^2}) \end{cases}$$

WLOG letting $A = 1$, we solve the above equation and find the tuple,

$$(A, B) = \left(1, \frac{-\Delta + \sqrt{\Delta^2 + t^2}}{t}\right), \quad \xrightarrow[\text{normalise}]{} \left(\frac{t}{\sqrt{2t^2 + 2\Delta^2 - 2\Delta\sqrt{\Delta^2 + t^2}}}, \frac{-\Delta + \sqrt{\Delta^2 + t^2}}{\sqrt{2t^2 + 2\Delta^2 - 2\Delta\sqrt{\Delta^2 + t^2}}}\right)$$

Thus, the first eigensystem we find would be,

$$\boxed{E_1 = E_0 + \sqrt{\Delta^2 + t^2}, \quad |\psi_1\rangle = \frac{t}{\sqrt{2t^2 + 2\Delta^2 - 2\Delta\sqrt{\Delta^2 + t^2}}} |a\rangle + \frac{-\Delta + \sqrt{\Delta^2 + t^2}}{\sqrt{2t^2 + 2\Delta^2 - 2\Delta\sqrt{\Delta^2 + t^2}}} |b\rangle}$$

Similarly, we can find the second eigensystem with the same procedure,

$$\begin{pmatrix} E_0 + \Delta & t \\ t & E_0 - \Delta \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = (E_0 - \sqrt{\Delta^2 + t^2}) \begin{pmatrix} A \\ B \end{pmatrix}, \quad \rightarrow \quad \begin{cases} A(E_0 + \Delta) + Bt &= A(E_0 - \sqrt{\Delta^2 + t^2}) \\ At + B(E_0 - \Delta) &= B(E_0 - \sqrt{\Delta^2 + t^2}) \end{cases}$$

WLOG letting $A = 1$, we solve the above equation and find the tuple,

$$(A, B) = \left(1, \frac{-\Delta - \sqrt{\Delta^2 + t^2}}{t}\right), \quad \xrightarrow[\text{normalise}]{} \left(\frac{t}{\sqrt{2t^2 + 2\Delta^2 + 2\Delta\sqrt{\Delta^2 + t^2}}}, \frac{-\Delta - \sqrt{\Delta^2 + t^2}}{\sqrt{2t^2 + 2\Delta^2 + 2\Delta\sqrt{\Delta^2 - t^2}}}\right)$$

Thus, the first eigensystem we find would be,

$$\boxed{E_2 = E_0 - \sqrt{\Delta^2 + t^2}, \quad |\psi_2\rangle = \frac{t}{\sqrt{2t^2 + 2\Delta^2 + 2\Delta\sqrt{\Delta^2 + t^2}}} |a\rangle + \frac{-\Delta - \sqrt{\Delta^2 + t^2}}{\sqrt{2t^2 + 2\Delta^2 + 2\Delta\sqrt{\Delta^2 + t^2}}} |b\rangle}$$

Taking the limit as $\Delta \to 0$, we see that the results here agree with part **b.**.

d. The probability of a wavefunction $|\psi\rangle$ to be localised in well a would be,

$$P(\text{localised in } a) = |\langle \psi | a \rangle|^2,$$

which is precisely the coefficient of $|a\rangle$ squared in the wavefunctions calculated above. We see, this probability can be written as,

$$|\langle \psi_{1,2} | a \rangle|^2 = \frac{t^2}{2t^2 + 2\Delta^2 \pm 2\Delta\sqrt{\Delta^2 + t^2}} = \frac{t^2(2t^2 + 2\Delta^2 \mp 2\Delta\sqrt{\Delta^2 + t^2})}{4t^4 + 4\Delta^2 + 8t^2\Delta^2 - 4\Delta^2(\Delta^2 + t^2)}$$

$$= \frac{t^2(2t^2 + 2\Delta^2 \mp 2\Delta\sqrt{\Delta^2 + t^2})}{4\Delta^2 t^2 + 4t^4} = \frac{2\Delta^2 t^2 + 2t^4 \mp 2\Delta t^2\sqrt{\Delta^2 + t^2}}{4\Delta^2 t^2 + 4t^4} = \frac{1}{2} \mp \frac{1}{2}\frac{\Delta t^2\sqrt{\Delta^2 + t^2}}{\Delta^2 t^2 + t^4}$$

$$= \frac{1}{2} \mp \frac{1}{2}\frac{\Delta\sqrt{\Delta^2 + t^2}}{\Delta^2 + t^2} = \frac{1}{2} \mp \frac{1}{2}\frac{(\Delta/t)}{\sqrt{1 + (\Delta/t)^2}}.$$

Since $\Delta, t > 0$, and our goal is to reach 90 percent, we must choose the eigenstate that gives us the positive sign, hence we will choose the eigenstate of the energy level,

$$\boxed{E_1 = E_0 + \sqrt{\Delta^2 + t^2}},$$

since its corresponding eigenvector gives the positive sign in the above calculation. Now, defining $\Delta/t = \eta$, if we want the probability to be greater than 90 percent, we write the equation,

$$P(\text{localised in } a) = \frac{1}{2} + \frac{1}{2}\frac{\eta}{\sqrt{1 + \eta^2}} = \frac{9}{10}$$

which solves to the condition,

$$\boxed{\eta = \frac{\Delta}{t} = \frac{4}{3}}$$

I   Formalism of Density Matrices

Now, we want to derive an alternate formalism of quantum mechanics that is able to handle key properties are are not exactly a characteristic of any particular eigenstates.

I.1   Pure and Mixed States

We will first define the **density operator** $\hat{\rho}$ of a state to be defined as follows.

Theorem 2.1: Definition of a Density Matrix

If $|\psi\rangle$ is a pure state, then the density operator associated with $|\psi\rangle$, denoted as $\hat{\rho}$, would be,

$$\hat{\rho} = |\psi\rangle \langle\psi|,$$

A pure state is a state where we know the state of the system without any ambiguity. A **mixed state** is, by contrast, a system where there is some uncertainty about the state, maybe because the system was interacting with another system that we didn't keep track of, or because it is in thermal contact with a bath, etc.

The matrix should be represented in a selected basis i (e.g. energy eigenstates). Once we have chosen a basis, we can define the matrix elements of the density matrix to be,

$$\hat{\rho}_{ij} = \langle i| \hat{\rho} |j\rangle = \langle i| \psi\rangle \langle\psi| j\rangle.$$

Similarly, if we take the matrix element of the opposite elements,

$$\hat{\rho}_{ji} = \langle j| \hat{\rho} |i\rangle = \langle j| \psi\rangle \langle\psi| i\rangle = \langle i| \hat{\rho} |j\rangle^{*}.$$

We have thus shown that the density operator is a Hermitian operator.

We can then look at what happens if we apply the density operator (for a pure state) twice,

$$\hat{\rho}^2_{\text{pure}} = |\psi\rangle \underbrace{\langle\psi| \psi\rangle}_{1} \langle\psi| = |\psi\rangle \langle\psi| = \hat{\rho}.$$

Now, we will define the **trace** of an operator as the sum of its diagonal elements,

$$\boxed{\text{Tr}\hat{A} \equiv \sum_i A_{ii}}.$$

We can compute the trace of the density operator to be,

$$\text{Tr}\rho = \sum_i \langle i| \hat{\rho} |i\rangle = \sum_i \langle i| \psi\rangle \langle\psi| i\rangle = 1$$

where this quantity is equal to one due to normalisation.

We can also look at the dynamics of the density operator. If we differentiate the density operator with respect to time, we see,

$$i\hbar \frac{d\hat{\rho}}{dt} = i\hbar \frac{d}{dt} \left(|\psi\rangle \langle\psi|\right) \xrightarrow[\text{product rule}]{=} i\hbar \left(\frac{d |\psi\rangle}{dt} \langle\psi| + |\psi\rangle \frac{d \langle\psi|}{dt} \right) = \left(i\hbar \frac{d |\psi\rangle}{dt} \right) \langle\psi| - |\psi\rangle \left(-i\hbar \frac{d \langle\psi|}{dt} \right)$$

$$= \hat{H} |\psi\rangle \langle\psi| + |\psi\rangle \left(\langle\psi| \hat{H} \right) = \hat{H}\hat{\rho} - \hat{\rho}\hat{H} = [\hat{H}, \hat{\rho}].$$

Therefore, we see that the time evolution of the density operator obeys the **von Neumann Equation**, as follows.

Theorem 2.2: The von Neumann Equation

$$i\hbar\frac{d\hat{\rho}}{dt} = \left[\hat{H}, \hat{\rho}\right]$$

Similarly, we can calculate the expected value of an observable via the equation as follows.

Theorem 2.3: Expected Value of Ensemble

$$\langle\hat{A}\rangle = \text{Tr}\left(\hat{\rho}\hat{A}\right).$$

Proof. Expanding the expression above into the contingent basis states, we see,

$$\text{Tr}\left(\hat{\rho}\hat{A}\right) = \text{Tr}\left(|\psi\rangle\langle\psi|\hat{A}\right) = \sum_i \langle i|\psi\rangle\langle\psi|\hat{A}|i\rangle = \sum_i \langle\psi|\hat{A}|i\rangle\langle i|\psi\rangle \xrightarrow[\text{resolving the identity}]{=} \langle\psi|\hat{A}|\psi\rangle,$$

which is the exact equation for expected values of pure states in the eigenstate formalism of quantum mechanics.

Now, we will try to extend the formalism of density matrices to mixed states. The **mixed-state density operator** is the probability-weighted sum of the density operators ρ_j for pure states as follows.

Theorem 2.4: Definition of Mixed-State Density Operator

$$\hat{\rho} = \sum_k P_k |\psi_k\rangle\langle\psi_k|$$

where the probability P_k is the probability for the system to be in each of the pure states. In other words, we think of an ensemble of systems, each in a pure state, but where we only know the probability that a given member of the ensemble is in a particular pure state.

This is extremely different from the superposition of pure states. In that case, we know exactly what the state of the system is, although we maybe don't know what result will occur from any given measurement. In a mixed state, by contrast, we have a set of probabilities for a set of pure states, where each of the pure states can of course be a superposition of different basis states.

The expected value of an operator due to a mixed state would naturally be a weighted probability of the expected value of the pure states,

$$\boxed{\langle\hat{A}\rangle = \sum_k P_k \langle\psi_k|\hat{A}|\psi_k\rangle.}$$

We can tell if a density operator is a mixed or a pure state by applying the density operator twice as follows.

> **Theorem 2.5: Pure or Mixed States**
>
> A density matrix $\hat{\rho}$ represents a pure state if and only if $\hat{\rho}^2 = \hat{\rho}$. If $\hat{\rho}^2 \neq \hat{\rho}$, then $\hat{\rho}$ represents a mixed state.

To better understand density matrices in general, it may be instructive to perform an example over spin-1/2 particles.

Example: Spin-1/2 Particles

In the z-spin basis, represented by the eigenkets $\{\ket{+\mathbf{z}}, \ket{-\mathbf{z}}\}$, the spin up and down states can be represented in matrix form as,

$$\ket{+\mathbf{z}} \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \ket{-\mathbf{z}} \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

The density matrix of a pure state with basis spin along $\hat{z}$ would therefore be,

$$\hat{\rho}_{+\mathbf{z}} = \ket{+\mathbf{z}}\bra{+\mathbf{z}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \frac{1 + \sigma_z}{2},$$

where σ_z is the z-component of the Pauli spin matrices. Similarly, the density matrix of the $\ket{-\mathbf{z}}$ state would be,

$$\hat{\rho}_{-\mathbf{z}} = \ket{-\mathbf{z}}\bra{-\mathbf{z}} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

Note that the two density matrices above satisfies the requirements for the density matrix of pure states, namely,

$$\hat{\rho}^2 = \hat{\rho}, \quad \mathrm{Tr}(\rho) = 1.$$

Now, the spins in the x direction would have a matrix representation in the $\{\ket{+\mathbf{z}}, \ket{-\mathbf{z}}\}$, as,

$$\ket{\pm\mathbf{x}} = \frac{\ket{+\mathbf{z}} \pm \ket{-\mathbf{z}}}{\sqrt{2}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}.$$

Therefore, the density matrices for the spin-x states would be,

$$\hat{\rho}_{+\mathbf{x}} = \ket{+\mathbf{x}}\bra{+\mathbf{x}} = \frac{1}{2} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \begin{pmatrix} 1 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = \frac{1 + \sigma_x}{2},$$

and similarly, for spin $-1/2$ in the x direction,

$$\hat{\rho}_{+\mathbf{x}} = \ket{-\mathbf{x}}\bra{-\mathbf{x}} = \frac{1}{2} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \begin{pmatrix} 1 & -1 \end{pmatrix} = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}.$$

Now, let's consider what happens if we are in a mixed state (an ensemble of spin-zs) with half of them being spin up and another half of them being spin down. The density matrix for this mixed state would therefore be,

$$\hat{\rho} = \underbrace{\frac{1}{2}}_{P_{\ket{+\mathbf{z}}}} \underbrace{\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}}_{\hat{\rho}_{\ket{+\mathbf{z}}}} + \underbrace{\frac{1}{2}}_{P_{\ket{-\mathbf{z}}}} \underbrace{\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}}_{\hat{\rho}_{\ket{-\mathbf{z}}}} = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{2} \mathbf{1}.$$

We clearly see that this matrix does not obey the properties of a pure state density matrix, as in, $\hat{\rho}^2 \neq \hat{\rho}$. However, we see that the trace of this (mixed) density matrix is still 1, $\mathrm{Tr}(\hat{\rho}) = 1$.

Now, let's try another example.

Purity of a Density Matrix

Naturally, we can define a quantity known as **purity** γ, which measures the degree to which a density matrix is mixed.

Theorem 2.6: Purity

The **purity** of a density matrix $\hat{\rho}$, which measures the degree to which a density matrix is mixed, can be defined as,
$$\gamma = \text{Tr}(\hat{\rho}^2).$$

When $\gamma = 1$, we see that $\text{Tr}(\hat{\rho}^2) = \text{Tr}(\hat{\rho}) = 1$, which implies that the density matrix is completely pure. However, let's consider an ensemble such that a probability of a of the system is in $|+\mathbf{z}\rangle$, while the probability of the system in $|-\mathbf{z}\rangle$ would be b. The total density matrix in this case would be,
$$\hat{\rho} = \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix}, \quad \rightarrow \quad \text{Tr}(\hat{\rho}^2) = a^2 + b^2.$$

Since we know that $a + b = 1$, the maximum value of $a^2 + b^2$ would simply be when $a = 1$ or $b = 1$, where there is no mixing at all. However, comparing values of (a, b) for, say, $(99.9\%, 0.1\%)$ versus $(50\%, 50\%)$, we clearly see that the latter has a lower $a^2 + b^2 = (0.5)^2 + (0.5)^2 = 0.5$ than the earlier $(0.99)^2 + (0.01)^2 \approx 1$. Therefore, we see, the higher the γ, the more "pure" our system is.

the Time-Evolution Operator and the Density Matrix

We can also describe the time evolution of the density matrix by applying an unitary operator, the time shift operator $\hat{U}(t, t_0)$,
$$\hat{U}(t, t_0) = \exp\left(-\frac{i}{\hbar}\hat{H}(t - t_0)\right).$$

If the Hamiltonian is time-independent, the von Neumann equation can be easily solved to yield,

$$\boxed{\hat{\rho}(t) = \exp\left(-\frac{i\hat{H}t}{\hbar}\right)\hat{\rho}(0)\exp\left(\frac{i\hat{H}t}{\hbar}\right).}$$

Proof. At a time $t = t_0$, a certain ensemble is represented by the density operator,
$$\hat{\rho}(0) = \sum_n A_n |\psi(0)\rangle \langle\psi(0)|$$

The time evolution of each state is represented by the time evolution operator,

$$|\psi(t)\rangle = \hat{U}(t, t_0) |\psi(t_0)\rangle = \exp\left(-\frac{i}{\hbar}\hat{H}(t - t_0)\right) |\psi(t_0)\rangle.$$

Therefore, the total time evolution of the ensemble would be,

$$\hat{\rho}(t) = \sum_n A_n |\psi(t)\rangle \langle\psi(t)| = \sum_n A_n \left[\exp\left(-\frac{i}{\hbar}\hat{H}(t - t_0)\right) |\psi(t_0)\rangle\right]\left[\langle\psi(t_0)| \exp\left(\frac{i}{\hbar}\hat{H}(t - t_0)\right)\right]$$

$$= \exp\left(-\frac{i}{\hbar}\hat{H}(t - t_0)\right)\left[\sum_n A_n |\psi(0)\rangle \langle\psi(0)|\right]\exp\left(\frac{i}{\hbar}\hat{H}(t - t_0)\right) = \hat{U}\hat{\rho}(0)\hat{U}^\dagger.$$

I.2   the Bloch Sphere

We can actually represent *all* spin-1/2 density matrices, pure or mixed states, in the form proposed as follows.

Theorem 2.7: Generalised Spin-1/2 States

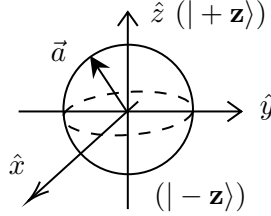$$\hat{\rho} = \frac{1}{2}\left(\mathbf{1} + \vec{a}\cdot\vec{\sigma}\right)$$

---

where $\vec{a}$ is the Bloch vector, and $\vec{\sigma}$ is the Pauli vector. The Bloch vector is a vector in the form,

$$\vec{a} = a_x\hat{x} + a_y\hat{y} + a_z\hat{z},$$

where its direction indicate the direction the spin[2]. The Pauli vector is simple, and simply is defined as,

$$\vec{\sigma} = \hat{\sigma}_x\hat{x} + \hat{\sigma}_y\hat{y} + \hat{\sigma}_z\hat{z},$$

where $\hat{\sigma}_i$ is the Pauli matrix in the i direction. Pictorially, we can visualise the Bloch sphere as follows.

The magnitude of the Bloch vector $\vec{a}$ represents how "mixed" my state is. $|\vec{a}| = 1$ indicate that our state is completely pure, while $|\vec{a}| = 0$ imply that our state is completely mixed.

Now, let's consider the mapping between $\hat{\rho}$ and $\vec{a}$. For the state $|+\mathbf{z}\rangle$, we see,

$$\hat{\rho}_{|+\mathbf{z}\rangle} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \hat{a} = \hat{z}.$$

Similarly, the down state would correspond to a density matrix and Bloch vector of,

$$\hat{\rho}_{|-\mathbf{z}\rangle} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad \hat{a} = -\hat{z}.$$

Now, as an example, the spin $+\hbar/2$ state in the x direction would have a density matrix and a Bloch vector of,

$$\hat{\rho}_{+|\mathbf{x}\rangle} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \quad \hat{a} = \hat{x}.$$

Problem 2.2: Spin in y Direction

Construct the density matrix for an electron that is either in the spin up along $\hat{y}$ (with

---

[2]Think of the direction of my Stern-Gerlach experiment.

> probability 1/5) or in the state spin down along $\hat{y}$ (with probability 4/5). Find $\langle \hat{S}_z \rangle$ and $\langle \hat{S}_x \rangle$ for the electron.

Solution. We do not know what the original state of the electron is, but we know that there is 1/5 probability it is $|+\mathbf{y}\rangle$ and $-4/5$ probability that it is $|-\mathbf{y}\rangle$. We know that the density matrix (in $|\pm\mathbf{z}\rangle$ basis) for all spin states can be expressed via the Bloch sphere,

$$\hat{\rho} = \frac{1}{2} \left(\mathbf{1} + \vec{a} \cdot \vec{\sigma} \right).$$

The state $|+\mathbf{y}\rangle$ will have a Bloch vector of $\hat{y}$, while the state $|-\mathbf{y}\rangle$ will have a Bloch vector of $-\hat{y}$. Therefore, we substitute the Bloch vectors to get the respective density of states for a pure $|+\mathbf{y}\rangle$ and $|-\mathbf{y}\rangle$ to be,

$$\hat{\rho} = \frac{1}{2} \left(\mathbf{1} + \hat{y} \cdot \vec{\sigma} \right) = \frac{1}{2} \left[\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \underbrace{\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}}_{\hat{\sigma}_y} \right] = \frac{1}{2} \begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix}.$$

Similarly, the density matrix for the state would be,

$$\hat{\rho} = \frac{1}{2} \left(\mathbf{1} - \hat{y} \cdot \vec{\sigma} \right) = \frac{1}{2} \left[\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \underbrace{\begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}}_{\hat{\sigma}_y} \right] = \frac{1}{2} \begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix}.$$

We then create the mixed state density matrix by a weighting of the pure states,

$$\hat{\rho}_{\text{mixed}} = \frac{1}{5}\hat{\rho} + \frac{4}{5}\hat{\rho} = \frac{1}{10} \begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} + \frac{4}{10} \begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix} = \boxed{\begin{pmatrix} 1/2 & 3i/10 \\ -3i/10 & 1/2 \end{pmatrix}}.$$

Note that this matrix is Hermitian, an the trace of this matrix is one.

We can calculate its expected value $\langle \hat{S}_z \rangle$ and $\langle \hat{S}_z \rangle$ via the expression, $\langle \hat{A} \rangle = \text{Tr}(\hat{\rho}\hat{A})$. We see,

$$\langle \hat{S}_z \rangle = \text{Tr}(\hat{\rho}\hat{S}_z) = \text{Tr}\left[\frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1/2 & 3i/10 \\ -3i/10 & 1/2 \end{pmatrix} \right] = \frac{\hbar}{2}\text{Tr}\left[\begin{pmatrix} 1/2 & 3i/10 \\ 3i/10 & -1/2 \end{pmatrix} \right] = \boxed{0}$$

$$\langle \hat{S}_x \rangle = \text{Tr}(\hat{\rho}\hat{S}_z) = \text{Tr}\left[\frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1/2 & 3i/10 \\ -3i/10 & 1/2 \end{pmatrix} \right] = \frac{\hbar}{2}\text{Tr}\left[\begin{pmatrix} -3i/10 & 1/2 \\ 1/2 & 3i/10 \end{pmatrix} \right] = \boxed{0}$$

These expected values make perfect sense since when we are in an eigenvalue of spin in the $\hat{y}$ direction, there is no spin in the other directions.

I.3 Spin-1/2 Particles in a Static Magnetic Field

Now, we can figure out the dynamics of spin-half particles due to an external magnetic field. The Hamiltonian due to an external magnetic field can be expressed as,

$$\hat{H} = g\hat{\mu} \cdot \vec{B},$$

where μ is the **magnetic dipole moment** due to the particle, and g is the magnitude of interaction, named the **g-factor for spin**. The magnetic dipole moment operator can be expressed as,

$$\hat{\mu} = \frac{\mu_B}{\hbar} \underbrace{\hat{S}}_{\text{spin operator}} \quad , \quad \hat{S} = \frac{\hbar}{2}\vec{\sigma} = \frac{\hbar}{2}\left(\hat{\sigma}_x\hat{x} + \hat{\sigma}_y\hat{y} + \hat{\sigma}_z\hat{z}\right)$$

where μ_B is the **Bohr magneton**, $\hat{\sigma}_i$ is the Pauli spin matrix in the i direction, and $\hat{i}$ is the unit vector in the direction of i.

If we assume that the magnetic field is in the $\hat{z}$ direction, as in, $\vec{B} = B_0\hat{z}$, the Hamiltonian can be rewritten as,

$$\boxed{\hat{H} = \frac{\mu_0 g}{2}B_0\hat{\sigma}_z}.$$

This interaction is called the **Zeeman interaction**, and it can split the degenerate energies of spin states into different quantities.
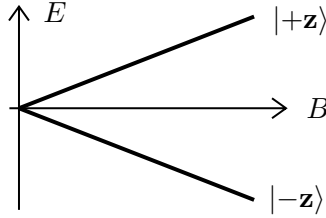
Now, we know that the density matrix of an ensemble of spin-1/2 particles will obey the expressions,

$$\hat{\rho} = \frac{1}{2}\left(\mathbf{1} + \vec{a}\cdot\vec{\sigma}\right), \quad i\hbar\frac{\partial\hat{\rho}}{\partial t} = \left[\hat{H}, \hat{\rho}\right].$$

To simplify the commutator, we evoke the identities,

$$[\hat{\heartsuit}, \mathbf{1}] = 0, \quad [\hat{\sigma}_i, \hat{\sigma}_j] = 2i\epsilon_{ijk}\hat{\sigma}_k.$$

Evoking the identities, the above equation therefore collapses into,

$$i\hbar\frac{\partial\hat{\rho}}{\partial t} = [\hat{H}, \hat{\rho}] = \frac{g\mu_B}{2}B_0\left[\hat{\sigma}_z, \frac{1}{2}\vec{\sigma}_a\cdot\vec{\sigma}\right].$$

Notice that even though our magnetic field lies in the z direction, we still have to take account of the evolution of the Bloch vector in three dimensions. However, the only thing that is time dependent in the density matrix is the projection of the $\vec{a}$ vectors. Thus, the above commutator relationship becomes,

$$\frac{i\hbar}{2}\left(\frac{\partial a_x}{\partial t}\hat{\sigma}_x + \frac{\partial a_y}{\partial t}\hat{\sigma}_y + \frac{\partial a_z}{\partial t}\hat{\sigma}_z\right) = \frac{2ig\mu_0 B_0}{4}\left(\underbrace{-a_x\hat{\sigma}_y + a_y\hat{\sigma}_x}_{[\hat{\sigma}_x, \hat{\sigma}_z]}\right).$$

Therefore, we can match the coefficients (of $\hat{\sigma}$s) to find that the equation above becomes three differential equations,

$$\frac{da_z}{dt} = 0, \quad \frac{da_x}{dt} = \frac{g\mu_B B_0}{\hbar}a_y, \quad \frac{da_y}{dt} = -\frac{g\mu_B B_0}{\hbar}a_x.$$

Eliminating one of the a_x or a_y components, we find that the above system can be simplified as,

$$\frac{d^2 a_x}{da_x^2} = \left(-\frac{g\mu_B B_0}{\hbar} \right)^2 a_x,$$

which we see that solves to,

$$a_x(t) = a_x(0) \cos\left(\frac{g\mu_B B_0}{\hbar} t \right), \quad a_y(t) = -a_y(0) \sin\left(\frac{g\mu_B B_0}{\hbar} t \right).$$

Since the parametric equations above trace out a circle, we see that,

$$a_x^2(t) + a_y^2(t) = a_x^2(0) + a_y^2(0) = \text{ constant.}$$

Therefore, the Bloch vector $\vec{a}$ is actually tracing a circle,

$$\boxed{\frac{d\vec{a}}{dt} = -\frac{g\mu_B}{\hbar} \vec{a} \times \vec{B}}.$$

The frequency of the precession, called **Larmor frequency**, can naturally be calculated to be,

$$\omega = \frac{g\mu_B B_0}{\hbar}.$$

The invariance of the magnitude of the Bloch vector also implies that the magnitude of "mixing" does not vary by time.
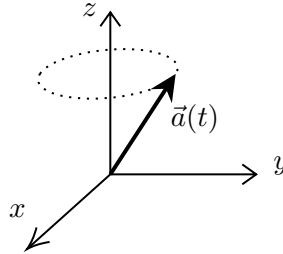

Theorem 2.8: Larmor Frequency

The precession of the Bloch vector about an external magnetic field has the **Larmor frequency** ω, quantified as,

$$\omega = \frac{g\mu_B B_0}{\hbar},$$

where B_0 is the magnitude of the external magnetic field orthogonal to the Bloch vector.

The resultant dynamics of the particle can be visualised by the figure below.

Expected Value for Spin Operators

Naturally, the expected values for spin operators should obey that of a general density matrix,

$$\langle \hat{S} \rangle = \text{Tr}(\hat{\rho}\hat{S}) = \text{Tr}\left(\frac{\mathbf{1} + \vec{a} \cdot \vec{\sigma}}{2} \cdot \frac{\hbar}{2}\vec{\sigma} \right).$$

Using the trace of Pauli spin matrices[3], as in,

$$\text{Tr}\hat{\sigma}_i = 0, \quad \text{Tr}(\hat{\sigma}_i\hat{\sigma}_j) = 2\delta_{ij} \quad \text{Tr}\hat{\sigma}_i^2 = 2,$$

we can evaluate the expected value of spin to be,

$$\langle\hat{S}\rangle = \frac{\hbar a_x}{4}\hat{x}\text{Tr}\hat{\sigma}_x^2 + \frac{\hbar a_y}{4}\hat{y}\text{Tr}\hat{\sigma}_y^2 + \frac{\hbar a_z}{4}\hat{z}\text{Tr}\hat{\sigma}_z^2.$$

All the traces of the $\hat{\sigma}^2$ components become 2, thus, the above expression and its time derivative becomes,

$$\langle\hat{S}\rangle = \frac{\hbar}{2}\vec{a}, \quad \frac{d\langle\hat{S}\rangle}{dt} = -\frac{g\mu_B}{\hbar}\langle\hat{S}\rangle \times \vec{B}.$$

I.4 Density Operator in the Singlet-Triplet Basis

Recall, from various previous derivations, that the total spin (and z-projections) forms a basis itself - we call this basis the **singlet-triplet basis**, where the basis vectors are written as follows. A **signlet** is a state of two spin-half particles such that the total system has total spin $s = 0$, as in,

$$|0,0\rangle \equiv |S\rangle = \frac{1}{\sqrt{2}}\left|\frac{1}{2},\frac{1}{2}\right\rangle_1\left|\frac{1}{2},-\frac{1}{2}\right\rangle_2 - \frac{1}{\sqrt{2}}\left|\frac{1}{2},-\frac{1}{2}\right\rangle_1\left|\frac{1}{2},\frac{1}{2}\right\rangle_2$$

Similarly, a **triplet** is a state with a total spin $s = 1$,

$$|1,1\rangle \equiv |T_+\rangle = \left|\frac{1}{2},\frac{1}{2}\right\rangle_1\left|\frac{1}{2},\frac{1}{2}\right\rangle_2$$

$$|1,0\rangle \equiv |T_0\rangle = \frac{1}{\sqrt{2}}\left|\frac{1}{2},\frac{1}{2}\right\rangle_1\left|\frac{1}{2},-\frac{1}{2}\right\rangle_2 + \frac{1}{\sqrt{2}}\left|\frac{1}{2},-\frac{1}{2}\right\rangle_1\left|\frac{1}{2},\frac{1}{2}\right\rangle_2$$

$$|1,-1\rangle \equiv |T_-\rangle = \frac{1}{\sqrt{2}}\left|\frac{1}{2},-\frac{1}{2}\right\rangle_1\left|\frac{1}{2},-\frac{1}{2}\right\rangle_2.$$

Conventionally, we express the density matrix of a two-particle state in singlet-triplet basis as follows,

$$\hat{\rho}_{1/2+1/2} = \begin{pmatrix} \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix} \begin{matrix} \rightarrow |S\rangle \\ \rightarrow |T_0\rangle \\ \rightarrow |T_+\rangle \\ \rightarrow |T_-\rangle \end{matrix}.$$
$$\begin{matrix} \downarrow & \downarrow & \downarrow & \downarrow \\ |S\rangle & |T_0\rangle & |T_+\rangle & |T_-\rangle \end{matrix}$$

To understand the singlet-triplet basis properly, we can consider the following example.

Problem 2.3: Two Spin-1/2 Particles in Singlet-Triplet Basis

This problem asks about the density matrix for two spin-1/2 particles in the singlet-triplet basis. Work with the quantisation axis along $\hat{z}$.

---

[3]Easily proven using brute force.

> **a.** What is the density matrix if the system has 50% probability of being the $|\uparrow\downarrow\rangle_z$ state and 50% probability for being in the $|\uparrow\uparrow\rangle_x$ state?
>
> **b.** For **a.**, what is the probability that the system is in the singlet state? In the $|T_0\rangle$ state?
>
> **c.** Introduce a zero-field spin splitting Δ for the triplet subsystem, which changes the relative energy of the $|T_0\rangle$ compared with the $|T_+\rangle$ and $|T_-\rangle$ states. Choose Δ such that the $|T_0\rangle$ state has the lowest energy. What is the Hamiltonian for this term in matrix form?

Solution.

a. First, we will express the two given states in terms of the singlet-triplet basis in the z direction. The $|\uparrow\uparrow\rangle_x$ corresponds to two spin particles pointing up in the x direction, which can be simplified into,

$$|\uparrow\uparrow\rangle_x = |+\mathbf{x}\rangle_1 |+\mathbf{x}\rangle_2 = \frac{1}{2} \left(|+\mathbf{z}\rangle_1 + |-\mathbf{z}\rangle_1 \right) \left(|+\mathbf{z}\rangle_2 + |-\mathbf{z}\rangle_2 \right)$$

$$= \frac{1}{2} |+\mathbf{z}\rangle_1 |+\mathbf{z}\rangle_2 + \frac{1}{2} |-\mathbf{z}\rangle_1 |+\mathbf{z}\rangle_2 + \frac{1}{2} |+\mathbf{z}\rangle_2 |-\mathbf{z}\rangle_1 + \frac{1}{2} |-\mathbf{z}\rangle_1 |-\mathbf{z}\rangle_2$$

$$= \frac{1}{2} |T_+\rangle + \frac{1}{\sqrt{2}} |T_0\rangle + \frac{1}{2} |T_-\rangle .$$

Similarly, the $|\uparrow\downarrow\rangle_z$ can be expressed in the singlet-triplet basis as,

$$|+\mathbf{z}\rangle_1 |-\mathbf{z}\rangle_2 = \frac{1}{\sqrt{2}} \left(|T_0\rangle + |S\rangle \right) .$$

Therefore, in the singlet-triplet basis representation, with $\mathcal{B} = \{|S\rangle, |T_0\rangle, |T_+\rangle, |T_-\rangle\}$, we will yield the matrix representations of $|\uparrow\uparrow\rangle_x$ and $|\uparrow\downarrow\rangle_z$ to be,

$$|\uparrow\uparrow\rangle_x = \begin{pmatrix} 0 \\ 1/\sqrt{2} \\ 1/2 \\ 1/2 \end{pmatrix}, \qquad |\uparrow\downarrow\rangle_z = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \\ 0 \end{pmatrix}.$$

Similarly, the pure-state density matrices representing the two states would be,

$$\hat{\rho}_{\uparrow\uparrow_x} = |\uparrow\uparrow\rangle_x \langle\uparrow\uparrow|_x = \begin{pmatrix} 0 \\ 1/\sqrt{2} \\ 1/2 \\ 1/2 \end{pmatrix} \begin{pmatrix} 0 & 1/\sqrt{2} & 1/2 & 1/2 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1/2 & 1/\sqrt{8} & 1/\sqrt{8} \\ 0 & 1/\sqrt{8} & 1/4 & 1/4 \\ 0 & 1/\sqrt{8} & 1/4 & 1/4 \end{pmatrix}.$$

Similarly, we see,

$$\hat{\rho}_{\uparrow\downarrow_z} = |\uparrow\downarrow\rangle_z \langle\uparrow\downarrow|_z = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} & 0 & 0 \end{pmatrix} = \begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

which, fortunately, both matrices obey the conditions of Hermiticity and normalisation, as in, $\mathrm{Tr}\rho = 1$. We can yield the mixed-state density matrix by weighing the probabilities of the ensemble

to be in either eigenstates,

$$\hat{\rho} = \frac{1}{2}\hat{\rho}_{\uparrow\uparrow x} + \frac{1}{2}\hat{\rho}_{\uparrow\downarrow z} = \frac{1}{2}\begin{pmatrix} 0 \\ 1/\sqrt{2} \\ 1/2 \\ 1/2 \end{pmatrix}\begin{pmatrix} 0 & 1/\sqrt{2} & 1/2 & 1/2 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1/2 & 1/\sqrt{8} & 1/\sqrt{8} \\ 0 & 1/\sqrt{8} & 1/4 & 1/4 \\ 0 & 1/\sqrt{8} & 1/4 & 1/4 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1/4 & 1/\sqrt{32} & 1/\sqrt{32} \\ 0 & 1/\sqrt{32} & 1/8 & 1/8 \\ 0 & 1/\sqrt{32} & 1/8 & 1/8 \end{pmatrix} + \begin{pmatrix} 1/4 & 1/4 & 0 & 0 \\ 1/4 & 1/4 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \boxed{\begin{pmatrix} 1/4 & 1/4 & 0 & 0 \\ 1/4 & 1/2 & 1/\sqrt{32} & 1/\sqrt{32} \\ 0 & 1/\sqrt{32} & 1/8 & 1/8 \\ 0 & 1/\sqrt{32} & 1/8 & 1/8 \end{pmatrix}},$$

which, fortunately, still obey the Hermiticity and normalisation condition.

b. The probability that a measurement of my ensemble will yield the *eigenstate* $|\psi\rangle$ can be expressed as,

$$P(|\psi\rangle) = \text{Tr}\left(\hat{P}_{|\psi\rangle}\hat{\rho}\right), \qquad \hat{P}_{|\psi\rangle} \equiv |\psi\rangle\langle\psi|.$$

In the singlet-triplet basis $\mathcal{B}$, the projection operators $\hat{P}_{|S\rangle}$ and $\hat{P}_{|T_0\rangle}$ can be expressed as,

$$\hat{P}_{|S\rangle} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \qquad \hat{P}_{|T_0\rangle} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

which then can be used in our calculation,

$$P(|S\rangle) = \text{Tr}\left(\hat{P}_{|S\rangle}\hat{\rho}\right) = \text{Tr}\left[\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1/4 & 1/4 & 0 & 0 \\ 1/4 & 1/2 & 1/\sqrt{32} & 1/\sqrt{32} \\ 0 & 1/\sqrt{32} & 1/8 & 1/8 \\ 0 & 1/\sqrt{32} & 1/8 & 1/8 \end{pmatrix}\right] = \text{Tr}\begin{pmatrix} 1/4 & 1/4 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \boxed{\frac{1}{4}}.$$

Similarly, we see,

$$P(|T_0\rangle) = \text{Tr}\left(\hat{P}_{|T_0\rangle}\hat{\rho}\right) = \text{Tr}\left[\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1/4 & 1/4 & 0 & 0 \\ 1/4 & 1/2 & 1/\sqrt{32} & 1/\sqrt{32} \\ 0 & 1/\sqrt{32} & 1/8 & 1/8 \\ 0 & 1/\sqrt{32} & 1/8 & 1/8 \end{pmatrix}\right]$$

$$= \text{Tr}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 1/4 & 1/2 & 1/\sqrt{32} & 1/\sqrt{32} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \boxed{\frac{1}{2}}.$$

c. The Hamiltonian, in the singlet-triplet basis, can be expressed as,

$$\boxed{\hat{H} = \begin{pmatrix} E_0 & 0 & 0 & 0 \\ 0 & E_0 - \Delta & 0 & 0 \\ 0 & 0 & E_0 & 0 \\ 0 & 0 & 0 & E_0 \end{pmatrix}},$$

where we mandate Δ to be real and positive such that the T_0 state has the lowest energy, while the other three energies are degenerate.

I.5   Partial Trace

Using the definition of trace,

$$\mathrm{Tr}\hat{\rho} = \sum_i \hat{\rho}_{ii} = \langle i|\,|\psi\rangle\,\langle\psi|\,|i\rangle,$$

we can define a similar concept called **partial trace**.

Often you have a system made up of different particles or subsystems. If we want to make measurements on one subsystem, without knowing anything about the rest of the system, how do we calculate this "partial measurement"? The answer is that you perform what is called a *partial trace* on the rest (unmeasured part) of the system, which will result in a density operator for the part of the system we do want to measure, from which you can calculate measurement outcomes.

Theorem 2.9: Partial Trace

The partial trace of a density matrix of a two particle system *over* particle 1 would be,

$$\mathrm{Tr}_1\left(\hat{\rho}_{1,2}\right) \equiv \sum_i \langle i|_1\,\hat{\rho}_{1,2}\,|i\rangle_1.$$

For example, we can consider a density matrix of a two spin-1/2 system. The partial trace over particle 1, in the $|\pm\mathbf{z}\rangle$ basis, would naturally be,

$$\mathrm{Tr}_1\hat{\rho}_{1,2} = \langle+\mathbf{z}|_1\hat{\rho}_{1,2}|+\mathbf{z}\rangle_1 + \langle-\mathbf{z}|_1\hat{\rho}_{1,2}|-\mathbf{z}\rangle_1.$$

Consider the following example cumulating our experience with density matrices.

Problem 2.4: Density Matrix of Constrained System

Consider a complete set of states, $|n\rangle$ and a system of two particles. Assume that, due to some physical restriction, $n_1 + n_2 = 3$ for $n_i > 1$.

   a. Write the most general state $|\psi\rangle$ for the two particles. What is the normalisation condition (constraints on the coefficients) for this state? What would be the corresponding density operator? Write this operator in matrix form.

   b. Since $\hat{\rho}$ is Hermitian and diagonalisable, what are the possible eigenvalues given that $\hat{\rho}^2 = \hat{\rho}$ and $\mathrm{Tr}\hat{\rho} = 1$?

   c. Consider now that we want to get the density matrix for the subsystem of particle 1, by summing over all possible results of physical measurements of the properties (n_2) of particle 2. That means, to consider the trace over states of particle 2. Write this matrix of the subsystem of particle 1 in terms of a 2 by 2 matrix, in the basis of the possible $|n_1\rangle$ states. What are the eigenvalues of this density matrix?

   d. The fact that I cannot specify the precise quantum state associated with particle 1 represents an uncertainty that is associated with entropy in this subsystem. Quantitatively, the *von Neuman entropy*, which measures the degree of purity of a quantum state, is de

---

ned mathematically as

$$S \equiv -\text{Tr}(\hat{\rho}\ln\hat{\rho}) = -\sum_i \lambda_i \ln(\lambda_i),$$

where λ_i are the eigenvalues of $\hat{\rho}$. Based on this definition, demonstrate that for a pure state, $S = 0$, while for mixed states $S \neq 0$. Evaluate it for the two cases consider above. When do we get the maximal value ? Present a short discussion on why this is the case.

Solution. Given that $n_{\min} = 1$ and $n_1 + n_2 = 3$, the possible basis for two $|n\rangle$ particles would be,

$$S = \{|1\rangle|1\rangle, |2\rangle|1\rangle, |1\rangle|2\rangle, |2\rangle|2\rangle\}.$$

a. The most general state $|\Psi\rangle$ for the two particles would be,

$$|\Psi\rangle = a|1\rangle|1\rangle + b|2\rangle|1\rangle + c|1\rangle|2\rangle + d|2\rangle|2\rangle.$$

However, we recognise that we want our total n to be 33, so the $|1\rangle|1\rangle$ and $|2\rangle|2\rangle$ state is nonexistent. Thus, our state with $n_1 + n_2 = 3$ would have the general state,

$$\boxed{|\Psi\rangle = a|2\rangle|1\rangle + b|1\rangle|2\rangle}$$

where the normalisation condition (constraints of the coefficients) would be,

$$\boxed{|a|^2 + |b|^2 = 1}.$$

The density matrix in the S basis would be,

$$\boxed{\hat{\rho} = |\Psi\rangle\langle\Psi| = \begin{pmatrix} 0 \\ a \\ b \\ 0 \end{pmatrix}(0, a^*, b^*, 0) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & aa^* & ab^* & 0 \\ 0 & ba^* & bb^* & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.}$$

$$\underbrace{\phantom{\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & aa^* & ab^* & 0 \\ 0 & ba^* & bb^* & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}}}_{|1\rangle|1\rangle, |2\rangle|1\rangle, |1\rangle|2\rangle, |2\rangle|2\rangle}$$

The square of the density matrix would be,

$$\hat{\rho}^2 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & aa^* & ab^* & 0 \\ 0 & ba^* & bb^* & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & aa^* & ab^* & 0 \\ 0 & ba^* & bb^* & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & aa^*aa^* + ab^*ba^* & aa^*ab^* + ab^*bb^* & 0 \\ 0 & ba^*aa^* + bb^*ba^* & ba^*ab^* + bb^*bb^* & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & aa^*(a^*a + b^*b) & ab^*(a^*a + b^*b) & 0 \\ 0 & ba^*(a^*a + b^*b) & bb^*(a^*a + b^*b) & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Using the normalisation condition,

$$aa^* + bb^* = 1,$$

the above density matrix becomes,

$$\hat{\rho}^2 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & aa^* & ab^* & 0 \\ 0 & ba^* & bb^* & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \hat{\rho}.$$

Similarly, we can compute the trace of this matrix to be,

$$\text{Tr}\rho = aa^* + bb^* = 1,$$

naturally following from the requirement for normalisation. We can also see the Hermiticity of the matrix by computing its Hermitian transpose,

$$\hat{\rho}^\dagger = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & (aa^*)^* & (ba^*)^* & 0 \\ 0 & (ab^*)^* & (bb^*)^* & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & a^*a & b^*a & 0 \\ 0 & a^*b & b^*b & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & (aa^*)^* & (ba^*)^* & 0 \\ 0 & (ab^*)^* & (bb^*)^* & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \hat{\rho}.$$

Thus, we see that all the properties of a pure state trace matrix has been obeyed.

b. The matrix must have determinant 1 since $\rho^2 = \rho$. Moreover, we know that a, b are less than 1 so their product of any a and b must be less than one. We recognise that the density matrix is Hermitian, so that it must have real eigenvalues. The only possible eigenvalues then would be, $\{-1, 0, 1\}$. However, we also know that the trace is invariant under all diagonalisation, so the sum of the eigenvalues must be one. Thus, we see that the -1 eigenvalue is impossible in an even Hilbert space. In this sense, we don't have to go to complex numbers, so the eigenvalues follow the two conditions,

$$\lambda = \boxed{0, 1}$$

c. We will be considering the basis $|n\rangle_1 = \{|1\rangle, |2\rangle\}$. We can compute the density matrix of the first state by summing the second particle via a partial trace,

$$\rho^{(1)} = \text{Tr}_2\hat{\rho}.$$

In other words, the reduced density operator for the subsystem of particle 1 would be,

$$\rho^{(1)} = \sum_j \langle\psi|_j\, \hat{\rho}\, |\psi\rangle_j = \langle 1|_2\, \hat{\rho}\, |1\rangle_2 + \langle 2|_2\, \hat{\rho}\, |2\rangle_2 = \langle 1|_2\, \hat{\rho}\, |1\rangle_2 + \langle 2|_2\, \hat{\rho}\, |2\rangle_2$$

$$= \langle 1|_2 \left[aa^* |2\rangle_1 |1\rangle_2 \langle 1|_2 \langle 2|_1 + bb^* |1\rangle_1 |2\rangle_2 \langle 2|_2 \langle 1|_1 \right] |1\rangle_2$$

$$+ \langle 2|_2 \left[aa^* |2\rangle_1 |1\rangle_2 \langle 1|_2 \langle 2|_1 + bb^* |1\rangle_1 |2\rangle_2 \langle 2|_2 \langle 1|_1 \right] |2\rangle_2$$

$$= \langle 1|_2\, aa^* |2\rangle_1 |1\rangle_2 \langle 1|_2 \langle 2|_1 |1\rangle_2 + \langle 1|_2\, bb^* |1\rangle_1 |2\rangle_2 \langle 2|_2 \langle 1|_1 |1\rangle_2$$

$$+ \langle 2|_2\, aa^* |2\rangle_1 |1\rangle_2 \langle 1|_2 \langle 2|_1 |2\rangle_2 + \langle 2|_2\, bb^* |1\rangle_1 |2\rangle_2 \langle 2|_2 \langle 1|_1 |2\rangle_2$$

$$= aa^* |2\rangle_1 \langle 2|_1 \left[\langle 1|_2 |1\rangle_2 \langle 1|_2 |1\rangle_2 \right] + bb^* |1\rangle_1 \langle 1|_1 \left[\langle 1|_2 |2\rangle_2 \langle 2|_2 |1\rangle_2 \right]$$

$$+ aa^* |2\rangle_1 \langle 2|_1 \left[\langle 2|_2 |1\rangle_2 \langle 1|_2 |2\rangle_2 \right] + bb^* |1\rangle_1 \langle 1|_2 \left[\langle 2|_2 |2\rangle_2 \langle 2|_2 |2\rangle_2 \right]$$

$$= aa^* |2\rangle_1 \langle 2|_1 + bb^* |1\rangle_1 \langle 1|_2$$

In matrix form, we see that $\hat{\rho}^{(1)}$ would be,

$$\boxed{\hat{\rho}^{(1)} = \underbrace{\begin{pmatrix} bb^* & 0 \\ 0 & aa^* \end{pmatrix}}_{|1\rangle_1 \langle 1|_1, |2\rangle_1, |2\rangle_1}}$$

This partial density matrix fulfills both trace condition,

$$\text{Tr}\hat{\rho}^{(1)} = bb^* + aa^* = 1,$$

while the square of the reduced density operator would be,

$$\hat{\rho}^{(1)2} = \begin{pmatrix} bb^* & 0 \\ 0 & aa^* \end{pmatrix} \begin{pmatrix} bb^* & 0 \\ 0 & aa^* \end{pmatrix} = \begin{pmatrix} bb^*bb^* & 0 \\ 0 & aa^*aa^* \end{pmatrix} \neq \hat{\rho}^{(1)}$$

Thus, the density matrix given above is not a pure state. The eigenvalues of this density matrix is simply,

$$\lambda = \boxed{bb^*, aa^*},$$

since the matrix given above is already diagonal.

d. The von Neumann entropy for a pure state would be,

$$S_{\text{pure}} = -\sum_i \lambda_i \ln(\lambda_i) = \sum_{\lambda=0} \lambda_i \ln(\lambda_i) + \sum_{\lambda=1} \lambda_j \ln(\lambda_j) = 0 + 0 = \boxed{0}.$$

$$S_{\text{mixed}} = \boxed{-bb^* \ln(bb^*) - aa^* \ln(aa^*)}.$$

We know that every term of $-\lambda \ln(\lambda_i)$ is less than 1 but greater than zero, since $\ln \lambda$ magnitude is in the order of greater than 1 for small numbers (as in, 0.01, etc); and λ is small. Therefore, I deire every term to be equal, which means every eigenvalue is equal, as in,

$$\lambda = \frac{\text{Tr}\rho}{N} = \frac{1}{N},$$

where N is the amount of basis states in the Hilbert space. Thus, we can then see that the von Neumann entropy would be,

$$\sum_N -\lambda_i \ln \lambda_i = \sum_N -\frac{1}{N} \ln \frac{1}{N} = \sum_N \frac{1}{N} \ln N = \left(\frac{1}{N} \ln N\right) N = \boxed{\ln N}.$$

I.6   Two-Particle Hamiltonians in the Singlet-Triplet Basis

In quantum engineering, one of the most important structures that we should be able to design would be those that preserve a quantum state for a very long time - effectively trying to implement *memory* into our qubit system.

However, it is evident that quantum particles would often interact with the outside environment and amongst themselves. Consider the **exchange Hamiltonian**, or the Hamiltonian that describes the energy that a particle feels when its near another particle, The exchange Hamiltonian can

position
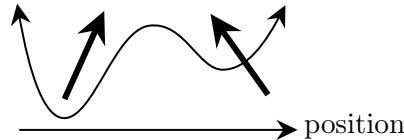
mathematically be described as,

$$\boxed{\hat{H}_{\text{exchange}} = J\hat{S}_1 \cdot \hat{S}_2},$$

where the constant J describes the *strength* of the interaction between the two particles. The exchange Hamiltonian arises from two major factors,

- **Overlap of the wavefunction**. The two electrons are no longer independent of each other.

- **Magnetic dipole interaction**. Treating each particle as infinitesimal magnets with one quanta, the magnetic fields of the particles will interact with each other.

We can eigenvalues of the dot product $\hat{S}_1 \cdot \hat{S}_2$ by considering the total angular momentum of the two particles, defined as,

$$\hat{S}_{\text{tot}} \equiv \hat{S}_1 + \hat{S}_2$$

Squaring the total angular momentum, we find,

$$\hat{S}_{\text{tot}}^2 = \hat{S}_1^2 + \hat{S}_2^2 + \underbrace{2\hat{S}_1 \cdot \hat{S}_2}_{[\hat{S}_1, \hat{S}_2]=0}, \quad \rightarrow \quad \hat{S}_1 \cdot \hat{S}_2 = \frac{\hat{S}_{\text{tot}}^2 - \hat{S}_1^2 - \hat{S}_2^2}{2}.$$

Working in the basis of the singlet-triplet state[4], we see,

$$\hat{S}^2 \left|T\right\rangle = (1)(1+1)\hbar^2 \left|T\right\rangle = 2\hbar^2 \left|T\right\rangle, \quad \hat{S}^2 \left|S\right\rangle = (0)(0+1)\hbar^2 \left|S\right\rangle = 0$$

$$\hat{S}_{1,2}^2 \left|T\right\rangle = (1/2)(1/2+1)\hbar^2 \left|T\right\rangle = \frac{3\hbar^2}{4} \left|T\right\rangle, \quad \hat{S}_{1,2}^2 \left|S\right\rangle = (1/2)(1/2+1)\hbar^2 \left|T\right\rangle = \frac{3\hbar^2}{4} \left|T\right\rangle.$$
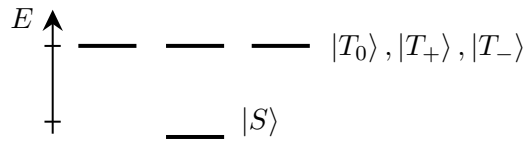
Therefore, we see that,

$$\begin{cases} \hat{S}_1 \cdot \hat{S}_2 \left|T\right\rangle = \dfrac{\hbar^2}{2}\left(2 - \dfrac{3}{4} - \dfrac{3}{4}\right) = \dfrac{\hbar^2}{4} \left|T\right\rangle \\ \hat{S}_1 \cdot \hat{S}_2 \left|S\right\rangle = \dfrac{\hbar^2}{2}\left(0 - \dfrac{3}{4} - \dfrac{3}{4}\right) = -\dfrac{3\hbar^2}{4} \left|S\right\rangle \end{cases}$$

Therefore, we can express the exchange Hamiltonian in the singlet-triplet basis as,

$$\boxed{\hat{H}_{\text{ex}} = -\frac{3J\hbar^2}{4} \left|S\right\rangle\left\langle S\right| + \sum_{i=+,-,0} \frac{J\hbar^2}{4} \left|T_i\right\rangle\left\langle T_i\right|.}$$

This means that there exists splitting of energy levels due to the exchange operator as follows. In

matrix form, the exchange Hamiltonian can be written as,

$$\hat{H}_{\text{eq}} = \begin{pmatrix} -\dfrac{3J\hbar^2}{4} & 0 & 0 & 0 \\ 0 & \dfrac{J\hbar^2}{4} & 0 & 0 \\ 0 & 0 & \dfrac{J\hbar^2}{4} & 0 \\ 0 & 0 & 0 & \dfrac{J\hbar^2}{4} \end{pmatrix}.$$

---

[4]The eigenstate of the angular momentum operator would be,

$$\hat{S}^2 \left|J\right\rangle = \hbar^2 j(j+1) \left|J\right\rangle.$$

In fact, exchange Hamiltonian $\hat{H}_{\text{ex}}$ is equivalent to the Pauli spin matrix $\hat{\sigma}_z$. Now, lets try another example to the spin-half composite system, where we apply a DC magnetic field to both of the spins. Here, we assume that the two spins have a different g-factor,

$$\hat{H} = \frac{g_1 \mu_B}{\hbar} \hat{S}_1 \cdot \vec{B} + \frac{g_2 \mu_B}{\hbar} \hat{S}_2 \cdot \vec{B}.$$

We can rewrite this Hamiltonian in the form,

$$\hat{H} = \left(\frac{g_1 + g_2}{2} \right) \frac{\mu_B}{\hbar} (\hat{S}_1 + \hat{S}_2) \vec{B} + \left(\frac{g_1 - g_2}{2} \right) \frac{\mu_B}{\hbar} (\hat{S}_1 - \hat{S}_2) \cdot \vec{B}.$$

What is especially interesting is the second half of the Hamiltonian - it can generate some nontrivial dynamics of the spin system. We single it out as the Δg Hamiltonian,

$$\hat{H}_{\Delta g} = \frac{\Delta g}{2} \frac{\mu_B}{\hbar} (\hat{S}_1 - \hat{S}_2) \vec{B}.$$

We can see what this Hamiltonian do to the singlet-triplet basis states,

$$\underbrace{(\hat{z} \cdot (\hat{S}_1 - \hat{S}_2)}_{2\hbar \hat{H}_{\Delta g}/\mu_B \Delta g} \left|+\mathbf{z}\right\rangle_1 \left|-\mathbf{z}\right\rangle_2 = \left(\frac{\hbar}{2} - \left(-\frac{\hbar}{2} \right) \right) \left|+\mathbf{z}\right\rangle_1 \left|-\mathbf{z}\right\rangle_2 = \hbar \left|+\mathbf{z}\right\rangle_1 \left|-\mathbf{z}\right\rangle_2,$$

$$\hat{z} \cdot (\hat{S}_1 - \hat{S}_2) \left|-\mathbf{z}\right\rangle_1 \left|+\mathbf{z}\right\rangle_2 = \left(-\frac{\hbar}{2} - \frac{\hbar}{2} \right) \left|-\mathbf{z}\right\rangle_1 \left|+\mathbf{z}\right\rangle_2 = -\hbar \left|-\mathbf{z}\right\rangle_1 \left|+\mathbf{z}\right\rangle_2.$$

Let's see what happens when we apply this Hamiltonian to the singlet state,

$$\hat{z} \cdot (\hat{S}_1 - \hat{S}_2) \left|S\right\rangle = \hbar \left(\frac{\left|+\mathbf{z}\right\rangle_1 \left|-\mathbf{z}\right\rangle_2 + \left|-\mathbf{z}\right\rangle_1 \left|+\mathbf{z}\right\rangle_2}{\sqrt{2}} \right) = \hbar \left|T_0\right\rangle.$$

Therefore, we see that the singlet state is no longer an eigenstate of the Δg Hamiltonian. Similarly, doing the same operator to $\left|T_0\right\rangle$, we find,

$$\hat{z} \cdot (\hat{S}_1 - \hat{S}_2) \left|T_0\right\rangle = \hbar S.$$

And, as derived previously, applying the Δg Hamiltonian to the two other triplet states would yield,

$$\hat{z}(\hat{S}_1 - \hat{S}_2) T_{\pm} = 0.$$

Therefore, we can again write the Δg Hamiltonian in matrix form[5],

$$\hat{H}_{\Delta g} = \frac{B_z \Delta g \mu_B}{2} \left(\left|T_0\right\rangle \left\langle S\right| + \left|S\right\rangle \left\langle T_0\right| \right) = \frac{\Delta g \mu_B B_z}{2} \hat{\sigma}_x,$$

which in *actual* matrix form, would be[6],

$$\hat{H}_{\Delta g} = \begin{pmatrix} 0 & \dfrac{B_z \Delta g \mu_B}{2} & 0 & 0 \\ \dfrac{B_z \Delta g \mu_B}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

We can make the following chart synthesising the similarities of the one spin-1/2 qubit and the two spin-1/2 singlet-triplet qubit.

---

[5] There seems to be homomorphism between the algebra of x-direction spin in the z basis and the algebra of $\left|S\right\rangle, \left|T_0\right\rangle$ states under the Δg Hamiltonian.

[6] Again, in the basis $\mathcal{B} = \{\left|S\right\rangle, \left|T_0\right\rangle, \left|T_+\right\rangle, \left|T_-\right\rangle\}$

	Spin-1/2 qubit	**Two spin-1/2 (singlet -triplet) qubit**
Diagonal $\hat{H}$	$B_z \to \hat{H} \propto B_z \hat{\sigma}_z$	$\hat{H}_{\text{ex}} = J\hat{S}_1\hat{S}_2$
Off-Diagonal $\hat{H}$	$B_x \to \hat{H} \propto B_x \hat{\sigma}_z \quad \leftrightarrow$	$\hat{H}_{\Delta g} = \dfrac{\Delta g\mu_B B_x}{2}(\hat{S}_1 - \hat{S}_2)$
Density Matrix	$\hat{\rho} = \begin{pmatrix} 0 & X \\ X & 0 \end{pmatrix}$	$\hat{\rho} = \begin{pmatrix} 0 & X \\ X & 0 \end{pmatrix}$
Basis	$\mathcal{B} = \{\lvert+\mathbf{z}\rangle, \lvert-\mathbf{z}\rangle\}$	$\mathcal{B} = \{\lvert S\rangle, \lvert T_0\rangle\}$

If spin-half systems can be qubits, there are is no reason why two spin-half systems (i.e. in the singlet-triplet basis) cannot be qubits too. In order to realise the two-spin-1/2 qubit, we often would choose two identical atoms and put them in a solid state environment. However, the lattice structure of the solid would create a magnetic gradient, therefore changing the effective g-factor for the two atoms. In this case, the two atoms can interact with each other using the Δg Hamiltonian.

II   Precession of Spin-1/2 Particles

In order to fully understand the effects of magnetic resonance, we need to evoke the Heisenberg picture of quantum mechanics.

The **Schrödinger picture** treats the wavefunction $\lvert\psi\rangle$ as time-dependent while the operator $\hat{\heartsuit}$ as time independent. On the contrary, the **Heisenberg picture** treats the wavefunction $\lvert\psi\rangle_H$ as time independent while the Heisenberg operator $\hat{\heartsuit}_H$ as time dependent. We can change between the Schrödinger and Heisenberg pictures of quantum mechanics using a unitary transformation change of basis,

$$\boxed{\hat{O}_H(t) = \exp\left(\frac{i\hat{H}t}{\hbar}\right)\hat{O}_S \exp\left(-\frac{i\hat{H}t}{\hbar}\right).}$$

### II.1   Interaction of Spin-1/2 Particles with a Magnetic Field

Now, we should try to apply the Heisenberg picture to the spin-1/2 particle in a magnetic field. The Hamiltonian and the time-evolution of the Bloch vector would look as follows,

$$\hat{H} = \frac{g\mu_B}{2}B_z\hat{\sigma}_z, \quad \frac{d\vec{a}}{dt} = -\frac{g\mu_B}{\hbar}\vec{a} \times \vec{B},$$

while the dynamics, as a review, would be a precession orthogonal to the magnetic field, as demonstrated below.

Let's say, we are interested in measuring the x-component of spin. We can rewrite the $\hat{S}_x$ operator in Heisenberg picture to be,

$$\hat{S}_{xH}(t) = \exp\left(\frac{i\omega_0 t}{2}\hat{\sigma}_z\right)\hat{S}_{xS}\exp\left(-\frac{i\omega_0 t}{2}\hat{\sigma}_z\right) = \hat{S}_x\cos(\omega_0 t) + \hat{S}_y\sin(_0 t).$$
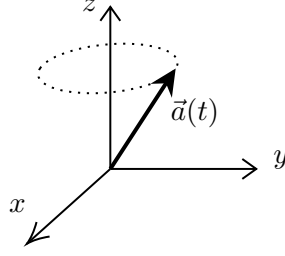
In[7] the Heisenberg picture, the Bloch vector $\vec{a}$ stays at $\vec{a}(0)$, while $\hat{S}_{xH}(t)$ keeps rotating at an angular frequency of ω_0.

AC Magnetic Field in the Rotated Basis

The Heisenberg picture makes applying an AC magnetic field, also known as **coherent driving**, a much simpler process. Now, consider not only if we have a DC magnetic field in the z-direction, we also have an AC magnetic field in the x direction, as depicted as follows.
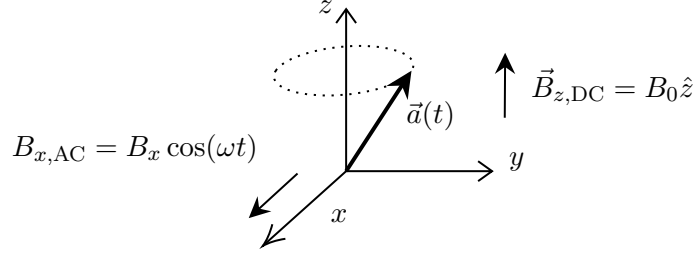
Note that the DC magnetic field causes the particle to already process around the z axis at an angular frequency of ω_0. The total Hamiltonian here would therefore be,

$$\hat{H} = \hat{H}_0 + \hat{H}_1, \qquad \boxed{\hat{H}_1 = \frac{g\mu_B}{2}B_1\cos(\omega t)\hat{S}_x}.$$

We can rewrite $B_x(t)$ as,

$$\boxed{B_x(t) = B_1\cos(\omega t)\hat{x} = \frac{1}{2}B_1\left(e^{i\omega t} + e^{-i\omega t}\right)\hat{x}},$$
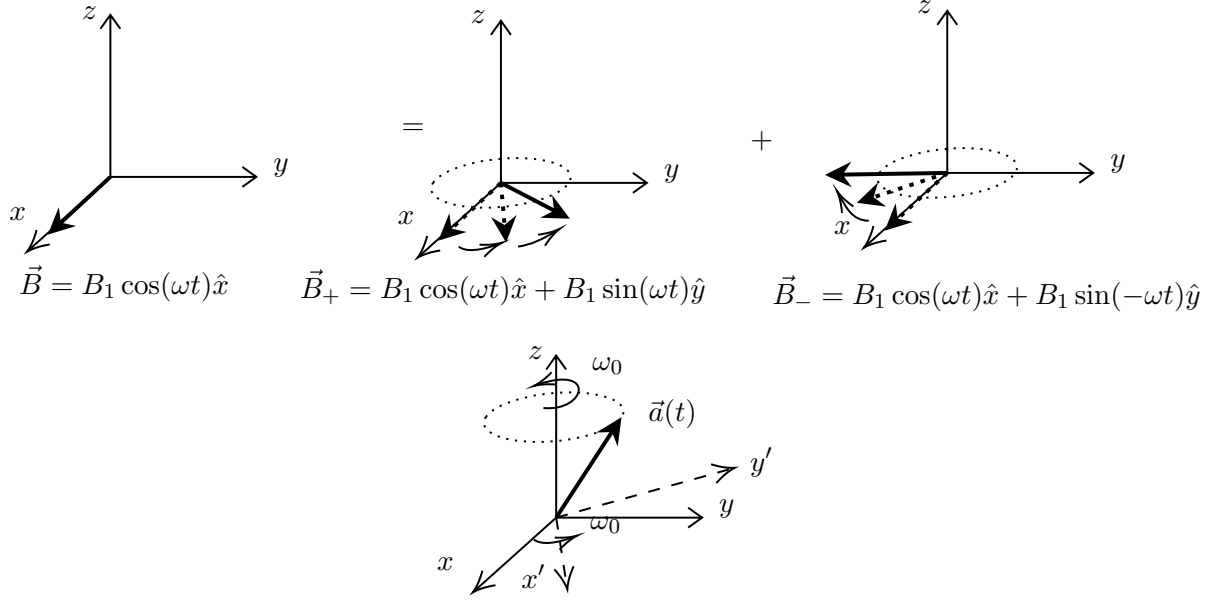
which is equivalent to $B_1/2$ rotating at $+\omega_z$ and $-\omega_z$ angular frequency about the z axis, as indicated in the figure below.

So far everything we have discussed was in the lab frame. However, it is easy for us to employ a rotating frame using the Heisenberg picture. We can choose our frame to rotate at ω_0, in order to cancel out the effect of Larmor precession due to the DC magnetic field.

---

[7]We can evaluate the expression above using a Taylor expansion for general spin rotations, where $\hat{n}$ is a normal vector of rotation

$$\exp\left(-\frac{i\omega t}{2}\hat{n}\cdot\hat{\sigma}\right) \xrightarrow[\theta \equiv \omega t]{} \exp\left(-\frac{i\theta}{2}\hat{n}\cdot\hat{\sigma}\right) = \cos\left(\frac{\theta}{2}\hat{n}\cdot\hat{\sigma}\right) - i\sin\left(\frac{\theta}{2}\hat{n}\cdot\hat{\sigma}\right)$$

$$= 1 - \frac{(\theta/2)^2(\hat{n}\cdot\hat{\sigma})^2}{2!} + \frac{(\theta/2)^4(\hat{n}\cdot\hat{\sigma})^4}{4!} + \cdots - i\sin\left(\frac{\theta}{2}\hat{n}\cdot\hat{\sigma}\right)$$

$$= \mathbf{1}\cos\left(\frac{\theta}{2}\right) - i\sin\left(\frac{\theta}{2}\right)\hat{n}\cdot\hat{\sigma}$$

since we know that the square of all Pauli matrices, $\hat{\sigma}_i^2$, will always be $\mathbf{1}$.

$$\vec{B} = B_1 \cos(\omega t)\hat{x} \qquad \vec{B}_+ = B_1 \cos(\omega t)\hat{x} + B_1 \sin(\omega t)\hat{y} \qquad \vec{B}_- = B_1 \cos(\omega t)\hat{x} + B_1 \sin(-\omega t)\hat{y}$$

From linear algebra one knows that a certain matrix $\mathbf{A}$ can be represented in another basis through the transformation

$$\mathbf{A}' = \mathbf{PAP}^{-1}$$

where $\mathbf{P}$ is the basis transformation matrix. Thus, we can actually rotate $\hat{H}^{(1)}$ into the basis where the particle is *stationary*, as in, the effects of Larmor precession about $\hat{z}$ is cancelled out. A rotation through an angle θ about the axis $\hat{n}$ is represented via the unitary transformation,

$$\hat{U} = \exp\left(\frac{i\theta\hat{n}\cdot\hat{\sigma}}{2}\right) = \mathbf{1}\cos\frac{\theta}{2} + i\hat{n}\cdot\hat{\sigma}\sin\frac{\theta}{2}.$$

For rotations about the z-axis, the above expression simplifies as,

$$\hat{U}_z = \mathbf{1}\cos\frac{\theta}{2} + i\hat{\sigma}_z\sin\frac{\theta}{2}.$$

Recall that $\hat{H}_1$ in the Schrödinger picture can be expressed as,

$$\hat{H}_1 = \frac{g\mu_B}{2}B_1\cos(\omega t) = \frac{g\mu_B}{2}\left[\frac{1}{2}B_1\left(e^{i\omega t} + e^{-i\omega t}\right)\hat{x}\right].$$

We can write the $\hat{H}_1$ operator in a rotating frame of ω_0, where ω_0 is the Larmor frequency due to the DC magnetic field in $\hat{z}$. Thus, the θ we will need to rotate would be $\omega_0 t$. This will therefore yield,

$$\hat{H}_{1,H} = \hat{R}(\omega_0 t)\hat{H}_{1,S}\hat{R}(\omega_0)^\dagger = \frac{g\mu_B B_1}{2\hbar}\left[\underbrace{\exp\left(\frac{i(\omega-\omega_0)t}{2}\hat{\sigma}_z\right)}_{\hat{P}}\hat{S}_{x,S}\underbrace{\exp\left(-\frac{i(\omega-\omega_0)t}{2}\hat{\sigma}_z\right)}_{\hat{P}^\dagger}\right] = \frac{g\mu_B B_1}{2\hbar}\hat{P}\hat{\sigma}_x\hat{P}^\dagger.$$

The **effective angular frequency** $\Delta\omega$ of the dynamics of $\hat{H}_{1,H}$ would therefore be, $\Delta\omega = \omega - \omega_0$ in this rotating frame. If we let $\Delta\omega$ to become zero, $\hat{H}_1$ in Heisenberg picture becomes,

$$\hat{H}_{1,H} = \frac{g\mu_B B_1}{2\hbar}\hat{S}_x,$$

which is time-independent. Note that the Hamiltonian above gone through the **rotating wave approximation**, which suggests the follows.

Theorem 2.10: Rotating Wave Approximation

In a resonance experiment with two systems, when we apply the **rotating wave approximation**, we can assume that the driving frequency ω is equal to the resonant frequency,

$$\omega = \omega_0 \text{ while } -\omega \neq \omega_0,$$

therefore the term with $\omega = \omega_0$ will die.

In essence, if we drive our external magnetic field at the Larmor frequency (ω_0), the external magnetic field would be stationary in the frame of the precessing particle due to the DC magnetic field. Recall that the quantum state after some time can be written as a time evolution operator as the form,

$$\boxed{|\psi(t = T)\rangle = \hat{U}(T) |\psi(t = 0)\rangle},$$

where $\hat{U}$ is a unitary operator known as the **time-evolution operator.** We can write the time evolution in the rotating frame using the time evolution operator,

$$\hat{U}(T) = \exp\left(\frac{i\hat{H}T}{\hbar}\right) = \exp\left(\frac{i}{\hbar} \frac{g\mu_B B_1}{2} \hat{S}_1 T\right)$$

which is precisely the form of the **rotation operator**.

Theorem 2.11: AC Magnetic Field at Resonant Frequency

In the rotating frame of reference, an AC magnetic field oscillating at the resonant (Larmor) frequency acts as a rotation operator,

$$\hat{U}(T) = \exp\left(\frac{i\hat{H}T}{\hbar}\right) = \exp\left(\frac{i}{\hbar} \frac{g\mu_B B_1}{2} \hat{S}_x T\right).$$

In other words, the AC magnetic field driving a spin-1/2 particle at resonant frequency corresponds to a **rotation** *about the x-axis* in the rotating frame where the Larmor precession is static.

As we have seen from the Larmor precession, this form of Hamiltonian would in fact induce a rotation about the x-axis at a frequency[8], in addition to the precession about z-axis that *looks stationary* in the reference frame. The precession frequency about x at this driving frequency $\omega = \omega_0$ would be,

$$\boxed{\Omega = \frac{g\mu_B B_1}{2\hbar}},$$

where this frequency is called the **Rabi frequency**. The AC magnetic field performs rotations of the spin vector along any axis, and the speed of that rotation is given by Ω. Consider the following figure describing the full dynamics combining DC and AC magnetic fields.

In essence, an addition of an AC magnetic field simply performs rotations of the spin vector along any axis, where the speed of rotation is given by Ω.
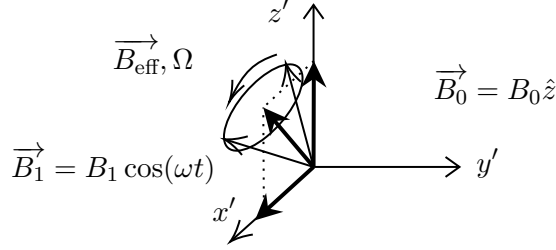
---

[8]in the rotating frame

Figure 2.1: In the rotating frame $x'y'z$, the effective field has a fixed direction, about which the spins rotate with a constant angular velocity.

II.2 Controlling Quantum States Using AC Magnetic Field Pulses

From the above analysis, we understand that the effect of AC magnetic fields can be encapsulated by unitary rotations *in the rotating frame* (or the interaction picture). All unitary rotations, by definition, can be expressed in the form,

$$\hat{U}_{\hat{n}}(\omega, t) = \exp\left(-\frac{i\omega t}{2}\hat{n}\cdot\hat{\sigma}\right).$$

Again, if we perform a Taylor expansion on the exponential above, we yield,

$$\exp\left(-\frac{i\theta}{2}\hat{n}\cdot\hat{\sigma}\right) = \cos\left(\frac{\theta}{2}\hat{n}\cdot\hat{\sigma}\right) - i\sin\left(\frac{\theta}{2}\hat{n}\cdot\hat{\sigma}\right) = \mathbf{1}\cos\left(\frac{\theta}{2}\right) - i\sin\left(\frac{\theta}{2}\right)\hat{n}\cdot\hat{\sigma}.$$

For example, the rotation unitary operator about the $\hat{x}$ axis would be,

$$\hat{U}_{\theta,x} = \begin{pmatrix} \cos\dfrac{\theta}{2} & -i\sin\dfrac{\theta}{2} \\ -i\sin\dfrac{\theta}{2} & \cos\dfrac{\theta}{2} \end{pmatrix}.$$

With this, we can now introduce **pulses** generated by the AC magnetic field. A $\pi-$**pulse** corresponds to applying an AC magnetic field such that a π rotation is introduced to the system (in the interaction picture). For instance, if we apply a π-pulse using the external magnetic field $B_1\cos(\omega t)\hat{x}$, the plot of the magnetic field would look as follows.
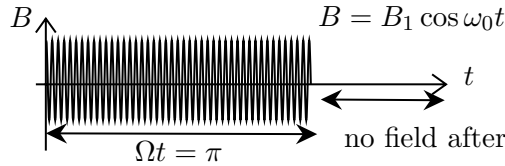
Similarly, a $\pi/\mathbf{2}$-**pulse** corresponds to applying an AC magnetic field such that a $\pi/2$ rotation is introduced. A $\pi/2$ pulse (about the x-axis) in matrix form looks like,

$$\hat{U}_{\pi/2,x} = \frac{1}{2}\begin{pmatrix} i & -i \\ -i & 1 \end{pmatrix},$$
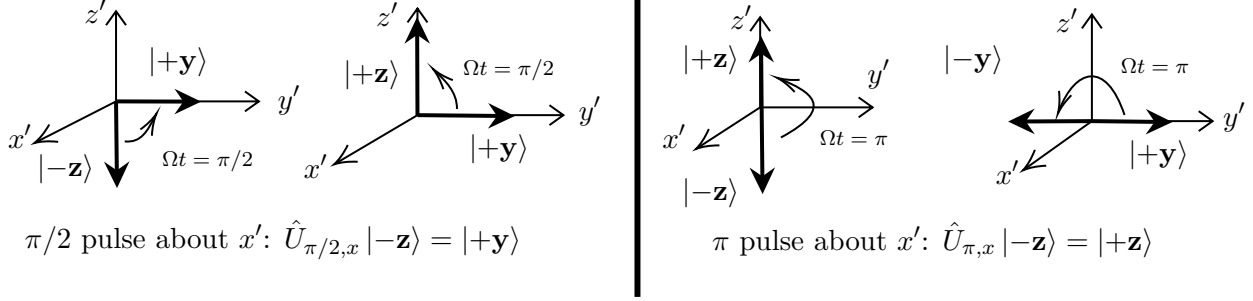
where, in the interaction frame, the $\pi/2$ pulse looks like,

$$\hat{U}_{\pi/2,x}\left|-\mathbf{z}'\right\rangle = \left|+\mathbf{y}'\right\rangle.$$

Similarly, we can represent the π-pulse as,

$$\hat{U}_{\pi,x} = -i \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = -\hat{\sigma}_x.$$

Geometrically, we can visualise a $\pi/2$ and π pulse as follows,

$\pi/2$ pulse about x': $\hat{U}_{\pi/2,x} \left|-\mathbf{z}\right\rangle = \left|+\mathbf{y}\right\rangle$ π pulse about x': $\hat{U}_{\pi,x} \left|-\mathbf{z}\right\rangle = \left|+\mathbf{z}\right\rangle$

However, since the rotation matrices were defined in the *rotating frame*, we need to transform the rotated Bloch vectors back to the lab frame. For instance, consider the transformation from $\left|+\mathbf{z}\right\rangle$ to $\left|+\mathbf{x}'\right\rangle$. If a Bloch vector is fixed in the x-axis in the rotating frame[9], the Bloch vector must therefore be rotating about the z axis on the xy plane in the fixed frame, as seen in the figure below.
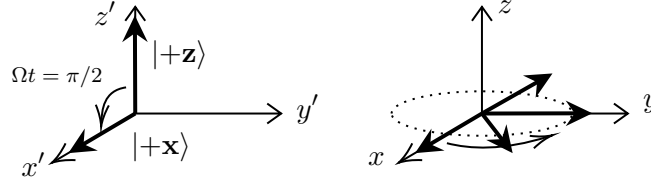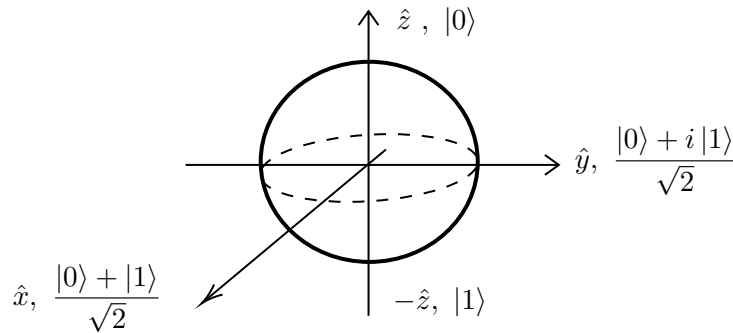

Connections to Quantum Computing

In quantum computing, we would typically use the $\left|+\mathbf{z}\right\rangle, \left|-\mathbf{z}\right\rangle$ states as qubits representing $\left|0\right\rangle$ and $\left|1\right\rangle$,

$$\boxed{\left|+\mathbf{z}\right\rangle, \left|-\mathbf{z}\right\rangle \leftrightarrow \left|1\right\rangle, \left|0\right\rangle}.$$

This can be represented on the Bloch vector **in the rotating frame** as follows,

---

[9]where the rotating frame itself is rotating about the z-axis at the Larmor frequency

If we apply a π-pulse onto a Bloch vector pointing in the $\hat{z}$ direction, since the rotating frame itself is rotating about the $\hat{z}$ direction, we know that the resultant rotation will be the same in both the fixed and the rotating frames. However, as seen above, if we apply a $\pi/2$ pulse onto the $|+\mathbf{z}\rangle$ state, the resultant Bloch vector would be one that rotates on the xy plane in the fixed frame.

Original $|+\mathbf{z}\rangle$ State $\pi/2$ Pulse (fixed) π Pulse (fixed)
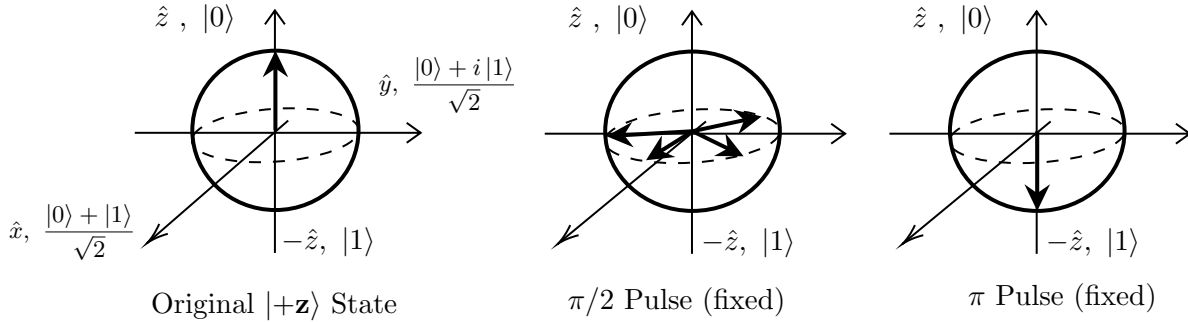
Therefore, we see that a π-pulse switches the qubit from a $|0\rangle$ state to $|1\rangle$ state, and vice versa. This is a physical realisation of the **NOT gate**. However, we see that it may be difficult to realise certain gates involving the $|\mathbf{x}\rangle$ and $|\mathbf{y}\rangle$ states due to the Larmor precession after a Rabi pulse. While we never turn off the static magnetic field in $\hat{z}$ that induces Larmor precession.

Why can implement quantum gates in the rotating frame?

Fortunately, in quantum computation, we always know the time-dependent phase factor due to the Larmor precession that makes the qubit precess in the fixed frame. In most cases, we can ignore that phase since it doesn't influence the measurement outcome. Moreover, all of the quantum gates that we use in quantum computing are defined in rotating frame. For instance, the Hadamard gate is defined such that,

$$|0\rangle \rightarrow \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle), \quad |1\rangle \rightarrow \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle),$$

or in the language of this chapter,

$$|+\mathbf{z}\rangle \rightarrow |+\mathbf{x}'\rangle, \quad |-\mathbf{z}\rangle \rightarrow |-\mathbf{x}'\rangle,$$

where x' is the x axis in the rotating frame. In quantum computing, the precise phase, or the γ term in the $\exp(i\gamma)$ term of the Bloch sphere, is not measurable - this property is called **phase invariance**. Therefore, the only thing that distinguishes the mapping $|0\rangle + |1\rangle$ and $|0\rangle - |1\rangle$ is really the relative phase shift between the two; the phase difference between two Bloch vectors will be conserved even if we view the two vectors in (the same) rotating frame. Therefore, we can see the follows,

> All quantum gates used in an NMR quantum computer[a] is defined in the rotating reference frame.
>
> ---
> [a]A quantum computer that utilises Rabi oscillations to move around the Bloch sphere.

II.3 Rabi Frequencies in General Two-Level Systems

In general, we often have to need to describe the dynamics of a quantum system undergoing a Hamiltonian in the form,

$$\hat{H} = \underbrace{\hat{H}_0}_{\text{static}} + \underbrace{\hat{H}_1}_{\text{sinusoidal}} .$$

The general strategy of dealing with the dynamics of two-state system goes as follows.

Step 1. Find the eigenbasis.

First, we consider what happens if the sinusoidal Hamiltonian $\hat{H}_1$ is non-existent. We want find the resonance frequency (ω_0) by first turning off the dynamic term[10]. The remaining Hamiltonian, $\hat{H}_0$, can be expressed in matrix form as,

$$\hat{H} = \hat{H}_0 = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \xrightarrow[\text{diagonalise}]{} \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix},$$

where we are now working in the eigenbasis of $\hat{H}_0$, denote to be $\mathcal{B} = \{|1\rangle, |2\rangle\}$. The **resonant frequency** due to this eigenbasis would be as follows.

> **Theorem 2.12: Resonant Frequency of a Hamiltonian**
>
> he resonant frequency needed to drive sinusoidally using a perturbing Hamiltonian $\hat{H}^{(1)}$ due to a system originally in the two-level Hamiltonian $\hat{H}^{(0)}$ would be,
>
> $$\omega_0 = \frac{E_1 - E_2}{\hbar},$$
>
> where E_1, E_2 are the eigenenergies of $\hat{H}^{(0)}$.

Step 2. Write the system in the eigenbasis.

To find the Rabi frequency, we are expected to work in this new basis $\mathcal{B}$ where $\hat{H}_0$ is diagonal. In this case, we can turn on the interaction Hamiltonian, which converts the *entire* Hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}_1$ into the eigenbasis of $\hat{H}^{(0)}$, and solve for the dynamics of the system in this eigenbasis.

> **Theorem 2.13: the Rabi Frequency**
>
> If there exists a Hamiltonian in the form $\hat{H} = \hat{H}^{(0)} + \hat{H}^{(1)}(t)$, the time-dependent part of the Hamiltonian, $\hat{H}^{(1)}$, can be expressed in the eigenbasis $\mathcal{B}$ of $\hat{H}^{(0)}$ in the form,
>
> $$\widetilde{\hat{H}^{(1)}} = \begin{pmatrix} 0 & \hbar\Omega\exp(i\omega t) \\ \hbar\Omega\exp(i\omega t) & 0 \end{pmatrix},$$
>
> where Ω, the **Rabi frequency**, is defined as,
>
> $$\Omega = \left| \frac{\text{off-diagonal term in } \mathcal{B}}{\hbar} \right|$$

---

[10]or, in the case of AC magnetic fields, turn off the AC field

> where, again, we are referring to the Hamiltonian **after** the rotating-wave approximation.

The term Ω is the **Rabi frequency**, or the frequency of precession in the rotating frame; we can also safely ignore the time-dependent terms simply by considering the Hamiltonian in an alternate picture[11]

---

[11]In the interaction picture of the rotating frame.