Two-Level System with Static and Dynamic Coupling

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Chapter 1

Two-State System

1.1 Two-State Hamiltonian

The wave function for a two state system can be written as a linear combination of two basis states

$$\psi(x,t) = c_1(t)\phi_1(x) + c_2(t)\phi_2(x) \tag{1.1}$$

where $\phi_1(x)$ and $\phi_2(x)$ are any complete basis states for the system. In particular, we can take the two basis states to be orthonormal so that

$$\langle \phi_i(x)|\phi_j(x)\rangle = \delta_{ij} \tag{1.2}$$

The time dependent coefficients satisfy the Schrödinger equation in matrix form

$$i\hbar \frac{d}{dt}\begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix} = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}\begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix} . \tag{1.3}$$

The matrix elements are given by

$$H_{ij} = \langle \phi_i(x)|\hat{H}|\phi_j(x)\rangle \tag{1.4}$$

1.2 Stationary Solutions: Eigen Functions and Eigen Energies

To find the stationary solutions (the eigen vectors) which are states of constant energy, so that the *eigen functions* are of the form

$$\begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix} = e^{-iEt/\hbar}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \tag{1.5}$$

Then the time-independent coefficients and energies are given by

$$\begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = E\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \tag{1.6}$$

There are two eigen energies given by the solutions to the determinant

$$\begin{vmatrix} H_{11} - E & H_{12} \\ H_{21} & H_{22} - E \end{vmatrix} = 0 \, . \tag{1.7}$$

Recall the fact that $H_{12} = H_{21}^*$, and we find

$$E_- = \frac{H_{11} + H_{22}}{2} - \sqrt{\left(\frac{H_{22} - H_{11}}{2}\right)^2 + |H_{12}|^2} \tag{1.8}$$

$$E_+ = \frac{H_{11} + H_{22}}{2} + \sqrt{\left(\frac{H_{22} - H_{11}}{2}\right)^2 + |H_{12}|^2} \tag{1.9}$$

Substitution of the eigen energies in the matrix equation (Eqn. 1.6) gives

$$\begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \begin{pmatrix} c_1^\pm \\ c_2^\pm \end{pmatrix} = E_\pm \begin{pmatrix} c_1^\pm \\ c_2^\pm \end{pmatrix} \tag{1.10}$$

which leads to

$$H_{21} c_1^\pm + (H_{22} - E_\pm) c_2^\pm = 0 \tag{1.11}$$

which results in the normalized solutions

$$\begin{pmatrix} c_1^\pm \\ c_2^\pm \end{pmatrix} = \frac{1}{\sqrt{1 + \left(\frac{H_{21}}{E_\pm - H_{22}}\right)}} \begin{pmatrix} 1 \\ \frac{H_{21}}{E_\pm - H_{22}} \end{pmatrix} \tag{1.12}$$

The algebra can be simplified by letting

$$\bar{E} = \frac{H_{11} + H_{22}}{2} \qquad \text{and} \qquad \Delta = \frac{H_{22} - H_{11}}{2} \tag{1.13}$$

and $H_{12} = H_{21}^* = V$. Then

$$\hat{H} = \begin{pmatrix} \bar{E} - \Delta & V \\ V^* & \bar{E} + \Delta \end{pmatrix} \tag{1.14}$$

and

$$E_- = \bar{E} - \sqrt{\Delta^2 + |V|^2} \tag{1.15}$$

$$E_+ = \bar{E} + \sqrt{\Delta^2 + |V|^2} \tag{1.16}$$

with eigen vectors

$$\begin{pmatrix} c_1^- \\ c_2^- \end{pmatrix} = \frac{1}{\sqrt{V^2 + \left(\Delta + \sqrt{\Delta^2 + V^2}\right)^2}} \begin{pmatrix} \Delta + \sqrt{\Delta^2 + V^2} \\ -V \end{pmatrix} = \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix} \tag{1.17}$$

and

$$\begin{pmatrix} c_1^+ \\ c_2^+ \end{pmatrix} = \frac{1}{\sqrt{V^2 + \left(-\Delta + \sqrt{\Delta^2 + V^2}\right)^2}} \begin{pmatrix} -\Delta + \sqrt{\Delta^2 + V^2} \\ +V \end{pmatrix} = \begin{pmatrix} -\sin\theta \\ \cos\theta \end{pmatrix} \tag{1.18}$$

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Figure 1.1: The eigen energy as a function of varying the coupling matrix element V. The wave functions are also indicated.

where

$$\sin 2\theta = -\frac{V}{\sqrt{\Delta^2 + V^2}} \qquad \text{and} \qquad \cos 2\theta = \frac{\Delta}{\sqrt{\Delta^2 + V^2}} \,. \tag{1.19}$$

Figs. 1.1 and 1.2 illustrate the eigen functions and the energies.

In summary, the eigen functions can be written in terms of the original basis set of ϕ_1 and ϕ_2 as

$$\psi_- = \cos\theta\,\phi_1 + \sin\theta\,\phi_2 \tag{1.20}$$

and

$$\psi_+ = -\sin\theta\,\phi_1 + \cos\theta\,\phi_2 \tag{1.21}$$

where

$$\sin 2\theta = -\frac{V}{\sqrt{\Delta^2 + V^2}} \qquad \text{and} \qquad \cos 2\theta = \frac{\Delta}{\sqrt{\Delta^2 + V^2}} \tag{1.22}$$

and, for convenience, $\Delta = (H_{22} - H_{11})/2$ and $V = V_{12}$ are taken as real. Also, we define the average unperturbed energy as $\bar{E} = (H_{22} + H_{11})/2$ and the energy difference as $\hbar\Omega = 2\sqrt{\Delta^2 + V^2}$, so that the eigen energies can be written as

$$E_\mp = \bar{E} \mp \hbar\Omega/2 \tag{1.23}$$

The general solution for the wave function at some time t, $\psi(t)$, is found from knowledge of the initial wave function $\psi(0)$, by writing $\psi(0)$ in terms of the eigen wave functions of the initial system ψ_- and ψ_+, and then evolving the wave function as

$$\psi(t) = c_-\psi_-e^{-iE_-t/\hbar} + c_+\psi_+e^{+iE_+t/\hbar}\,, \tag{1.24}$$

where $c_- = \langle\psi_-|\psi(0)\rangle$ and $c_+ = \langle\psi_+|\psi(0)\rangle$.

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Figure 1.2: The eigen energy as a function of varying the energy difference matrix element Δ. The wave functions are also indicated.

Oscillations between states

Suppose the system is originally in state $\Psi(x, 0) = \phi_1(x)$, which is not an eigen state of the system. Then $c_- = \cos\theta$ and $c_+ = -\sin\theta$. Hence,

$$\psi_1(t) = \left[\cos^2\theta\, e^{-iE_-t/\hbar} + \sin^2\theta\, e^{-iE_+t/\hbar}\right]\phi_1 + \sin\theta\cos\theta\left[e^{-iE_-t/\hbar} - e^{-iE_+t/\hbar}\right]\phi_2. \quad (1.25)$$

The probability of being in state 2 is

$$p_2(t) = 4\sin^2\theta\cos^2\theta\sin^2\sqrt{\Delta^2 + V^2}\, t/\hbar \qquad (1.26)$$

Use that $2\sin\theta\cos\theta = \sin^2 2\theta$, and

$$p_2(t) = \frac{V^2}{\Delta^2 + V^2}\sin^2\sqrt{\Delta^2 + V^2}\, t/\hbar \qquad (1.27)$$

Therefore, we can write

$$p_2(t) = \frac{1}{2}\frac{V^2}{\Delta^2 + V^2} - \frac{1}{2}\frac{V^2}{\Delta^2 + V^2}\cos 2\sqrt{\Delta^2 + V^2}\, t/\hbar \qquad (1.28)$$

and

$$p_1(t) = \frac{1}{2}\frac{2\Delta^2 + V^2}{\Delta^2 + V^2} + \frac{1}{2}\frac{V^2}{\Delta^2 + V^2}\cos 2\sqrt{\Delta^2 + V^2}\, t/\hbar \qquad (1.29)$$

Hence the dynamics of the system is that one state oscillates into the other state with frequency

$$\Omega = 2\sqrt{\Delta^2 + V^2}/\hbar \qquad (1.30)$$

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Figure 1.3: Probabilities as a function of time states 1 and 2, for given values of Δ/V, note that time is in units of $\hbar/V$.

while the time-averaged the probability in each state is

$$\langle p_1 \rangle = \frac{1}{2} \frac{2\Delta^2 + V^2}{\Delta^2 + V^2} \qquad \text{and} \qquad \langle p_2 \rangle = \frac{1}{2} \frac{V^2}{\Delta^2 + V^2} \tag{1.31}$$

These probabilities are shown in Fig. 1.3

In the case with $\Delta = 0$ the eigenvectors are determined by θ; in this limit, we obtain

$$\cos\theta = \sin\theta = \frac{1}{\sqrt{2}} \tag{1.32}$$

This is equivalent to the statement that the new states ψ_- and ψ_+ are made up of equal amounts of the original basis states ϕ_1 and ϕ_2. In this limit, the probabilities become

$$p_1 \longrightarrow \cos^2 \frac{|V|t}{\hbar} = \frac{1 + \cos\left(\frac{2|V|t}{\hbar}\right)}{2} \tag{1.33}$$

and

$$p_2 \longrightarrow \sin^2 \frac{|V|t}{\hbar} = \frac{1 - \cos\left(\frac{2|V|t}{\hbar}\right)}{2} \tag{1.34}$$

The transfer of probability between states ϕ_1 and ϕ_2 now becomes total. The frequency of transitions, $\Omega = 2|V|/\hbar$, is now determined completely by the strength of the coupling $|V|$; this is an important limit that has observable and useful consequences. (Note that the frequency at which the probability changes is twice that of the frequency of the probability amplitudes, since the probability is the square of the amplitudes.)

For example, When

$$\Omega t = \frac{2|V|t}{\hbar} = \pi \tag{1.35}$$

then $p_1(t) = 0$ and $p_2(t) = 1$, so that the state has completely changed from the lower state to the upper state. The sequence is often called a π-pulse. If we call the lower state $|0\rangle$ and the upper state $|1\rangle$, then we can say that the π-pulse has changed the state $|0\rangle$ to the state $|1\rangle$. If we further associate a logical "0" with $|0\rangle$ and a logical "1" with $|0\rangle$, then the π-pulse can be said to implement a NOT logical operation. Indeed if the initial state were $|1\rangle$ then the π-pulse would have converted it into the state $|0\rangle$. Associating logical states with quantum states forms the basis for quantum logic and quantum computation. The physical system that embodies these two states is referred to as a quantum bit or a qubit.

In general there are other logical operations that can be done on the two state system. We now discuss how these logical state operations can be identified with a quantum mechanical operator.

1.3   Evolution as a Unitary Operator

In the previous section a solution for the wave function at some time t, $\psi(t)$, was found from knowledge of the initial wave function $\psi(0)$, by writing $\psi(0)$ in terms of the eigen wave functions of the initial system ψ_- and ψ_+, and then evolving the wave function

$$\psi(t) = c_-\psi_- e^{-iE_- t/\hbar} + c_+\psi_+ e^{+iE_+ t/\hbar} \,, \tag{1.36}$$

where $c_- = \langle \psi_- | \psi(0) \rangle$ and $c_+ = \langle \psi_+ | \psi(0) \rangle$. The eigen functions can be written in terms of the original basis set of ϕ_1 and ϕ_2 as

$$\psi_- = \cos\theta \, \phi_1 + \sin\theta \, \phi_2 \tag{1.37}$$

and

$$\psi_+ = -\sin\theta \, \phi_1 + \cos\theta \, \phi_2 \tag{1.38}$$

where

$$\sin 2\theta = -\frac{V}{\sqrt{\Delta^2 + V^2}} \qquad \text{and} \qquad \cos 2\theta = -\frac{\Delta}{\sqrt{\Delta^2 + V^2}} \tag{1.39}$$

and, for convenience, $\Delta = (H_{22} - H_{11})/2$ and $V = V_{12}$ are taken as real. Also, we define the average unperturbed energy as $\bar{E} = (H_{22} + H_{11})/2$ and the energy difference as $\hbar\Omega = 2\sqrt{\Delta^2 + V^2}$, so that the eigen energies can be written as

$$E_{\mp} = \bar{E} \mp \hbar\Omega/2 \tag{1.40}$$

For example, it was shown that if the initial state is $\psi(0) = \phi_1$, then

$$\psi_1(t) = \left[\cos^2\theta \, e^{-iE_- t/\hbar} + \sin^2\theta \, e^{-iE_+ t/\hbar}\right]\phi_1 + \sin\theta\cos\theta\left[e^{-iE_- t/\hbar} - e^{-iE_+ t/\hbar}\right]\phi_2 \,. \tag{1.41}$$

Similarly, if the initial state is $\psi(0) = \phi_2$, then

$$\psi_2(t) = \left[\sin^2\theta \, e^{-iE_- t/\hbar} + \cos^2\theta \, e^{-iE_+ t/\hbar}\right]\phi_2 + \sin\theta\cos\theta\left[e^{-iE_- t/\hbar} - e^{-iE_+ t/\hbar}\right]\phi_1 \,. \tag{1.42}$$

In general, if the initial state is any arbitrary state, $\psi(0) = a\phi_1 + b\phi_2$, then the time dependent state is simply $\psi(t) = a\psi_1(t) + b\psi_2(t)$, which in terms of ϕ_1 and ϕ_2 is a complicated expression. To make the solution more compact, we denote the wave function as

$$\psi(t) = c_1(t)\phi_1 + c_2(t)\phi_2 \tag{1.43}$$

and write the state as

$$|\psi(t)\rangle = \begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix} , \tag{1.44}$$

Then by combining the above equations, we find

$$\begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix} = U(t) \begin{pmatrix} a \\ b \end{pmatrix} . \tag{1.45}$$

where the evolution matrix is

$$U(t) = e^{-i\bar{E}t/\hbar} \begin{pmatrix} \cos^2\theta e^{i\Omega t/2} + \sin^2\theta e^{-i\Omega t/2} & \sin\theta\cos\theta(e^{i\Omega t/2} - e^{-i\Omega t/2}) \\ \sin\theta\cos\theta(e^{i\Omega t/2} - e^{-i\Omega t/2}) & \sin^2\theta e^{i\Omega t/2} + \cos^2\theta e^{-i\Omega t/2} \end{pmatrix} . \tag{1.46}$$

The matrix $U(t)$ can be further simplified by taking the zero of energy to be $\bar{E}$, (that is, the overall phase factor does not enter in evaluating any physical state),

$$U(t) = \begin{pmatrix} \cos\Omega t/2 + i\cos 2\theta \sin\Omega t/2 & i\sin 2\theta \cos\Omega t/2 \\ i\sin 2\theta \cos\Omega t/2 & \cos\Omega t/2 - i\cos 2\theta \sin\Omega t/2 \end{pmatrix} . \tag{1.47}$$

The evolution matrix has the interesting property that $U(t)U^\dagger(t) = 1$, that is $U^{-1}(t) = U(t)^\dagger$ and such a matrix is known as a *unitary matrix*. Hence, we say that the evolution is unitary.

The property of unitary evolution is, in fact, general. If some $\Psi(t) = U(t)\Psi(0)$, and the normalization of the wave function remains constant during its evolution, then $\langle\Psi(0)|\Psi(0)\rangle = \langle\Psi(t)|\Psi(t)\rangle$. But since

$$\langle\Psi(t)|\Psi(t)\rangle = \langle\Psi(0)U(t)|U(t)\Psi(0)\rangle = \langle\Psi(0)(U(t)^\dagger U(t))\Psi(0)\rangle \tag{1.48}$$

we must demand that $U^{-1}(t) = U^\dagger(t)$.

Now let's see how to write the NOT operation in terms of a matrix operator. Recall that the operation occurred when $\Delta = 0$ so that $\Omega = 2|V|/\hbar$ and $\sin 2\theta = -V$ and $\cos 2\theta = 0$. For simplicity, we take an attractive potential $V = -|V|$. At this point,

$$U(t) = \begin{pmatrix} \cos|V|t/\hbar & i\sin|V|t/\hbar \\ i\sin|V|t/\hbar & \cos|V|t/\hbar \end{pmatrix} \tag{1.49}$$

What was needed for a π-pulse is that such that $\Omega = 2|V|t/\hbar = \pi$. (Again the relevant frequency is for the probability and not the probability amplitudes.) The evolution matrix becomes

$$U_\pi = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} . \tag{1.50}$$

Now let U_π operate on the logical qubit states,

$$U_\pi \begin{pmatrix} 1 \\ 0 \end{pmatrix} = i \begin{pmatrix} 0 \\ 1 \end{pmatrix} \qquad \text{and} \qquad U_\pi \begin{pmatrix} 0 \\ 1 \end{pmatrix} = i \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{1.51}$$

or equivalently,

$$U_\pi|0\rangle = i|1\rangle \qquad \text{and} \qquad U_\pi|1\rangle = i|0\rangle \tag{1.52}$$

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Figure 1.4: $E - \bar{E}$ vs. Delta

Therefore, we can identified the NOT operator as

$$\text{NOT} = -iU_\pi = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{1.53}$$

What one would like to do is to start the state in the ground state $|0\rangle$, and then after some operation, keep it in a state such that the probability of it being in the new state remains the same in time. One way to accomplish this is to consider the energy eigenvalues as a function of the energy difference Δ as shown in Fig. 1.4. When $\Delta = 0$ the eigen energies are $-|V|$ and $|V|$ with respective eigen states of $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$. When $\Delta \gg |V|$, then the eigen energies are $-\Delta$ and Δ with respective eigen states $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$. In many quantum systems the value of Δ corresponds to the classical energy difference of two states and it can be controlled. For example, in a system with two small capacitors through which electrons can also tunnel, the energy difference Δ between states can be changed rapidly by changing the applied voltage [1]. In systems with loops of superconducting Josephson junctions, Δ can be changed rapidly by changing the magnetic flux through the loop. [2]

To perform the NOT operation, start the system with $\Delta \gg |V|$, so that the ground state is $|0\rangle$. Then rapidly reduce Δ to zero, and let the system evolve there for the π-pulse duration t_π, and then change $\Delta \gg |V|$ so that the system will evolve in time with the eigen states $|0\rangle$ and $|1\rangle$ retaining the same probability. For example, after the full operation the wave function will evolve as $|\psi(t)\rangle = e^{-i\Delta(t-t_\pi)/\hbar}|1\rangle$. The system then remains in the $|1\rangle$ state.

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[1] Y. Nakamura, Y.A. Pashkin, J.S. Tsai, " Coherent control of macroscopic quantum states in a single-Cooper-pair box" *Nature* **398**, 786—788, (1999).

[2] Caspar H. van der Wal, A. C. J. ter Haar, F. K. Wilhelm, R. N. Schouten, C. J. P. M. Harmans, T. P. Orlando, Seth Lloyd, and J. E. Mooij, "Quantum Superposition of Macroscopic Persistent-Current States," Science, 290, 773 (2000). Also, Science 285, 1036 (1999); and J. R. Friedman, Vijay Patel, W. Chen, S. K. Tolpygo and J. E. Lukens, "Quantum Superposition of Distinct Macroscopic States," Nature 406, p.43, (2000).

Another operation is the Hadamard transformation, U_H,

$$U_H|0\rangle = \frac{1}{2}\left(|0\rangle + |1\rangle\right) \tag{1.54}$$

which takes the $|0\rangle$ state and produces an equally weighted combination of states. The Hadamard operation is important because it allows one to produce a linear combination of states, to which a new logical operation can be performed on both "bits" at the same time. It is this quantum parallelism with underlies the speed up for some operations in quantum computation.

How are we to produce U_H? First start the system in the $|0\rangle$ by setting $\Delta \gg |V|$ and letting the system settle to the ground state. (Here we assume that if we wait a long enough time known as the relaxation time the system will settle to its ground state due to dissipation through its interaction with other states in its environment. We will discuss this process in more detail in Section 25.9.) Then quickly change $\Delta = 0$ and let the system evolve for a $\Omega t_1 = \pi/2$ which is known as as $\pi/2$-pulse. The pulse occurs in a time $t_1 = \pi\hbar/4|V|$, for which

$$U_{\Delta=0}(t_1) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix} \tag{1.55}$$

The state is now $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}$. Now switch the state back to $\Delta \gg |V|$, and let it evolve for a time $t_2 = \pi\hbar/4|\Delta|$, for which

$$U_{\Delta\gg|V|}(t_2) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1+i & 0 \\ 0 & 1-i \end{pmatrix} \tag{1.56}$$

so that the state becomes

$$\psi(t_1 + t_2) = \frac{1+i}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1+i}{2}\left(|0\rangle + |1\rangle\right) \tag{1.57}$$

which to within a phase factor is the desired state. Finally, note that the result is the same as cascading the operations,

$$|\psi(t_1 + t_2)\rangle = U_{\Delta\gg|V|}(t_2)U_{\Delta=0}(t_1)|0\rangle \tag{1.58}$$

so that processes that builds up more complex logical operations (or evolution) can be represented by a product of unitary transformations which is itself a unitary transformation.

1.4   Density Operator Approach

The two-state system has given us two ways to envision the time-dependence of the wave function. First by solving the differential equation in time and matching boundary conditions, and second by finding the time-evolution operator as a matrix which propagates the coefficients basis states in time. In both cases the physical quantities of interest are usually the average values of operators, such as position or momentum or energy. A third method is now presented which focuses directly on the coefficients used in calculating the average values. This method, known as the density matrix approach is useful is solving

some problems, but more importantly, it will be used in latter chapters when statistical mechanics is discussed and when dissipation is needed to describe a quantum system.

In terms of the basis states ϕ_1 and ϕ_2, the wave function is

$$\psi(t) = c_1(t)\phi_1 + c_2(t)\phi_2 \,. \tag{1.59}$$

The average value of any operator $\hat{O}$ can be written as

$$\begin{aligned}
\langle \hat{O} \rangle = \quad & c_1(t)c_1^*(t) \, \langle \phi_1|\hat{O}|\phi_1 \rangle + c_2(t)c_1^*(t) \, \langle \phi_1|\hat{O}|\phi_2 \rangle \\
+ \quad & c_1(t)c_2^*(t) \, \langle \phi_2|\hat{O}|\phi_1 \rangle + c_2(t)c_2^*(t) \, \langle \phi_2|\hat{O}|\phi_2 \rangle
\end{aligned} \tag{1.60}$$

Again we denote the wave function as a column vector and write the state as

$$|\psi(t)\rangle = \begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix} \,. \tag{1.61}$$

The density matrix is then defined as

$$\hat{\rho} = |\psi(t)\rangle\langle\psi(t)| = \begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix} \begin{pmatrix} c_1^*(t) & c_2^*(t) \end{pmatrix} \tag{1.62}$$

which in terms of the coefficients is

$$\hat{\rho} = \begin{pmatrix} c_1(t)c_1^*(t) & c_1(t)c_2^*(t) \\ c_2(t)c_1^*(t) & c_2(t)c_2^*(t) \end{pmatrix} \tag{1.63}$$

The density matrix then satisfies $\rho_{11} + \rho_{22} = 1$ and $\rho_{12}^* = \rho_{21}$. Recall that the operator $\hat{O}$ can be represented as the matrix

$$\hat{O} = \begin{pmatrix} \langle \phi_1|\hat{O}|\phi_1 \rangle & \langle \phi_1|\hat{O}|\phi_2 \rangle \\ \langle \phi_2|\hat{O}|\phi_1 \rangle & \langle \phi_2|\hat{O}|\phi_2 \rangle \end{pmatrix} \tag{1.64}$$

The average value of the operator can then be written as the trace of the matrix product as

$$\langle \hat{O} \rangle = \mathrm{tr}\left(\hat{\rho}\hat{O} \right) \,. \tag{1.65}$$

The trace is the sum of the diagonal components of a matrix, $\mathrm{tr}(A) = \sum_i A_{ii}$

The equations for time dependence of elements of the density matrix can be found explicitly. With the chain rule,

$$\frac{d}{dt}\hat{\rho} = \left[\frac{d}{dt}\begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix} \right] \begin{pmatrix} c_1^*(t) & c_2^*(t) \end{pmatrix} + \begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix} \frac{d}{dt}\begin{pmatrix} c_1^*(t) & c_2^*(t) \end{pmatrix} \,. \tag{1.66}$$

With the use of Schrödinger's equation

$$i\hbar\frac{d}{dt}\begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix} = \hat{H}\begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix} \qquad \text{and} \qquad -i\hbar\frac{d}{dt}\begin{pmatrix} c_1^*(t) & c_2^*(t) \end{pmatrix} = \begin{pmatrix} c_1^*(t) & c_2^*(t) \end{pmatrix}\hat{H} \tag{1.67}$$

one finds

$$\frac{d}{dt}\hat{\rho} = -\frac{1}{i\hbar}\left[\hat{\rho}, \hat{H} \right] \,. \tag{1.68}$$

Note the sign difference between this relationship and Ehrenfest's theorem.

Let's consider the general Hamiltonian written as

$$\hat{H} = \begin{pmatrix} \bar{E} - \Delta & V \\ V^* & \bar{E} + \Delta \end{pmatrix} \tag{1.69}$$

Eqn. 2.5 gives

$$\frac{d}{dt} \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix} = \begin{pmatrix} \rho_{12}V^* - \rho_{21}V & (\rho_{11} - \rho_{22})V + 2\rho_{12}\Delta \\ (\rho_{22} - \rho_{11})V - 2\rho_{21}\Delta & \rho_{21}V - \rho_{12}V^* \end{pmatrix} \tag{1.70}$$

In principle, this is a system of 8 equations for 8 real unknowns, the real and imaginary parts of each ρ_{ij}. But since ρ_{11} is real, $\rho_{22} = 1 - \rho_{11}$, and $\rho_{12} = \rho_{21}^*$, there are only three independent real variables. One useful set of the three independent real quantities is

$$N(t) = \rho_{22} - \rho_{11} \tag{1.71}$$

and

$$Q(t) = \rho_{21} + \rho_{12} \tag{1.72}$$

and

$$P(t) = \frac{1}{i}(\rho_{21} - \rho_{12}). \tag{1.73}$$

Here $N(t)$ is the population difference between the upper and the lower states. The real part of the off-diagonal part of the density matrix is $Q(t)$ and the imaginary part is $P(t)$.

The equations of motion for each of these are

$$\frac{d}{dt}N(t) = -\frac{1}{i\hbar}\left\{Q(t)(V - V^*) + iP(t)(V + V^*)\right\} \tag{1.74}$$

and

$$\frac{d}{dt}Q(t) = \omega_o P(t) + \frac{1}{i\hbar}N(t)(V - V^*) \tag{1.75}$$

and

$$\frac{d}{dt}P(t) = -\omega_o Q(t) + \frac{1}{\hbar}N(t)(V + V^*) \tag{1.76}$$

where $\omega_o = 2\Delta/\hbar$. These three coupled equations are known as the Bloch Equations. For completeness, the average value of the operator is

$$\begin{aligned} \langle \hat{O} \rangle &= \frac{1}{2}\left[\langle \phi_1|\hat{O}|\phi_1\rangle + \langle \phi_2|\hat{O}|\phi_2\rangle\right] + \frac{1}{2}\left[\langle \phi_2|\hat{O}|\phi_2\rangle - \langle \phi_1|\hat{O}|\phi_1\rangle\right]N(t) \\ &\quad + Q(t)\text{Re}\left\{\langle \phi_1|\hat{O}|\phi_2\rangle\right\} + iP(t)\text{Im}\left\{\langle \phi_1|\hat{O}|\phi_2\rangle\right\} \end{aligned} \tag{1.77}$$

Let's solve the above three coupled Bloch equations for the case where V is real and the initial values of $N(0)$, $Q(0)$ and $P(0)$ are known. The equations become

$$\frac{d}{dt}N(t) = -\frac{2V}{\hbar}P(t) \tag{1.78}$$

and

$$\frac{d}{dt}Q(t) = \omega_o P(t) \tag{1.79}$$

and

$$\frac{d}{dt}P(t) = -\omega_o Q(t) + \frac{2V}{\hbar}N(t)\,. \tag{1.80}$$

Taking the time derivative of the equation for $P(t)$, one finds

$$\frac{d^2}{dt^2}P(t) = -\Omega^2 P(t) \tag{1.81}$$

where

$$\Omega = \sqrt{\omega_o^2 + \left(\frac{2V}{\hbar}\right)^2}\,. \tag{1.82}$$

Therefore, $P(t)$ is a sum of sinusoids at frequency Ω. Therefore, to match the initial condition on $P(t)$ and its derivative (Eqn. 1.80),

$$P(t) = P(0)\cos\Omega t + \left[\frac{2V}{\hbar\Omega}N(0) - \frac{\omega_o}{\Omega}Q(0)\right]\sin\Omega t\,. \tag{1.83}$$

Now $Q(t)$ and $N(t)$ can be found by integrating Eqns. 1.79 and 1.78 to give

$$Q(t) = \frac{\omega_o P(0)}{\Omega}\sin\Omega t - \frac{\omega_o}{\Omega}\left[\frac{2V}{\hbar\Omega}N(0) - \frac{\omega_o}{\Omega}Q(0)\right](\cos\Omega t - 1) + Q(0)\,. \tag{1.84}$$

and

$$N(t) = -\frac{2V P(0)}{\hbar\Omega}\sin\Omega t + \frac{2V}{\hbar\Omega}\left[\frac{2V}{\hbar\Omega}N(0) - \frac{\omega_o}{\Omega}Q(0)\right](\cos\Omega t - 1) + N(0)\,. \tag{1.85}$$

As an example, let the wave function is initially in the ϕ_1 state that is, $\begin{pmatrix}1\\0\end{pmatrix}$, then $N(0) = -1$, $Q(0) = 0$ and $P(0) = 0$. Furthermore, let $\Delta = 0$ so $\Omega = 2V/\hbar$, then

$$N(t) = -\cos 2Vt/\hbar \qquad \text{and} \qquad P(t) = -\sin 2Vt/\hbar \qquad \text{and} \qquad Q(t) = 0\,. \tag{1.86}$$

Equivalently, $|c_1(t)|^2 = \cos^2 Vt/\hbar$ and $|c_2(t)|^2 = \sin^2 Vt/\hbar$ as expected for the states to oscillate fully back and forth at the $\Delta = 0$ point.

1.5   Two-level system with dynamical coupling

The dynamics of the two level system are much richer in the event that the coupling between the states is time-dependent. We are only able to get exact solutions for a simple sinusoidal potential. In general, we are no longer able to obtain exact solutions as above, since the equations are much more difficult to solve. Yet an understanding of the resulting dynamics is important for applications in a variety of different areas, including NMR, laser physics, quantum information, and other applications where the simple models are relevant. We will first recall the equation of motion for the density matrix approach and solve the sinusoidal driving problem. Then we will discuss the solutions for the wave functions and the unitary evolution matrix. Lastly, we will make some observations about the general time-dependent problem.

1.5.1   Including the dynamical coupling

As before we denote the wave function as a linear combination of basis states

$$\psi(t) = c_1(t)\phi_1 + c_2(t)\phi_2 \tag{1.87}$$

where the time dependent coefficients satisfy the matrix equation

$$i\hbar \frac{d}{dt}\begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix} = \begin{pmatrix} \bar{E} - \Delta & V(t) \\ V^*(t) & \bar{E} + \Delta \end{pmatrix}\begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix}. \tag{1.88}$$

The dynamics of the system can also be written in terms of the time evolutions of the density matrix (Eqn. 1.70), or equivalently in terms of the three independent real variable as the Bloch equations

$$\frac{d}{dt}N(t) = -\frac{1}{i\hbar}\left\{Q(t)(V - V^*) + iP(t)(V + V^*)\right\} \tag{1.89}$$

and

$$\frac{d}{dt}Q(t) = \omega_o P(t) + \frac{1}{i\hbar}N(t)(V - V^*) \tag{1.90}$$

and

$$\frac{d}{dt}P(t) = -\omega_o Q(t) + \frac{1}{\hbar}N(t)(V + V^*) \tag{1.91}$$

where $\omega_o = 2\Delta/\hbar$. We e can also solve the problem with the other methods of finding the equations of motion for the coefficients of the wave functions and also finding the unitary evolution operator. However, we will first focus on solving the problem with the Bloch equations because in this case these equations can be mapped onto the well-known problem in classical dynamics of a magnetic moment in a magnetic field. Then we will comment briefly on the other two methods, leaving the detail of these two methods to be worked out as problems.

1.5.2   Sinusoidal driving potential

Consider the simple, but instructive case, of applying to the two-level system a sinusoidal potential $V(t) = Ve^{i\omega t}$, where V is real. This simulates a case of two energy levels separated by energy $2\Delta = \hbar\omega_o$ excited by a radiation field at frequency ω. We expect that we can cause transitions between the two levels if the driving frequency is equal to or near the energy difference. The Bloch equations become

$$\frac{d}{dt}Q(t) = \omega_o P(t) + \frac{2V}{\hbar}\sin\omega t\, N(t) \tag{1.92}$$

and

$$\frac{d}{dt}P(t) = -\omega_o Q(t) + \frac{2V}{\hbar}\cos\omega t\, N(t) \tag{1.93}$$

and

$$\frac{d}{dt}N(t) = -\frac{2V}{\hbar}\cos\omega t\, P(t) - \frac{2V}{\hbar}\sin\omega t\, Q(t) \tag{1.94}$$

These coupled equations can be reduced to the form of the previous time independent problem by the following. Define the vectors

$$\mathbf{M}(t) = Q(t)\mathbf{i}_x + P(t)\mathbf{i}_y - N(t)\mathbf{i}_z \tag{1.95}$$

and

$$\gamma\mathbf{B}(t) = -\frac{2V}{\hbar}\left(\cos\omega t\mathbf{i}_x - \sin\omega t\mathbf{i}_y\right) + \omega_o\mathbf{i}_z\,. \tag{1.96}$$

Then the Bloch equations can be written as

$$\frac{d}{dt}\mathbf{M}(t) = \mathbf{M}(t) \times \gamma\mathbf{B}(t)\,. \tag{1.97}$$

This is just the equation for the dynamics of the magnetization in the presence of a static magnetic field in the z-directions and an oscillating field in the xy-plane. This equation is best solved by going to reference frame which rotates with frequency $-\omega$ about the z-axis. The time derivative of any vector is its time derivative in the rotating frame plus the oscillating part, that is,

$$\frac{d}{dt}\mathbf{M}(t) = \frac{\partial}{\partial t}\mathbf{M}'(t) - \omega\mathbf{i}_z \times \mathbf{M}'(t)\,. \tag{1.98}$$

where $\mathbf{M}'(t)$ is the vector in the rotating frame

$$\mathbf{M}'(t) = Q'(t)\mathbf{i}'_x + P'(t)\mathbf{i}'_y - N'(t)\mathbf{i}_z\,. \tag{1.99}$$

Also in the rotating frame

$$\gamma\mathbf{B}'(t) = -\frac{2V}{\hbar}\mathbf{i}'_x + \omega_o\mathbf{i}_z\,. \tag{1.100}$$

Combining the above equations, we find in the rotating frame

$$\frac{\partial}{\partial t}\mathbf{M}'(t) = \mathbf{M}'(t) \times \left[\frac{2V}{\hbar}\mathbf{i}'_x + (\omega_o - \omega)\mathbf{i}_z\right]\,. \tag{1.101}$$

This yields the three equations

$$\frac{\partial}{\partial t}Q'(t) = (\omega_o - \omega)P'(t) \tag{1.102}$$

and

$$\frac{\partial}{\partial t}P'(t) = -(\omega_o - \omega)Q'(t) + \frac{2V}{\hbar}N'(t)\,. \tag{1.103}$$

and

$$\frac{\partial}{\partial t}N'(t) = -\frac{2V}{\hbar}P'(t)\,. \tag{1.104}$$

These three equations are of the same form as the time independent problem given by Eqns. 1.79, 1.80, and 1.78, but with $\omega_o - \omega$ replacing ω_o. Therefore, the solutions for $Q'(t)$, $P'(t)$, and $N'(t)$ are the same as for the Eqns. 1.4, 1.83, and 1.85,

$$P'(t) = P(0)\cos\Omega t + \left[\frac{2V}{\hbar\Omega}N(0) - \frac{\omega_o - \omega}{\Omega}Q(0)\right]\sin\Omega t\,. \tag{1.105}$$

and

$$Q'(t) = \frac{(\omega_o - \omega)P(0)}{\Omega} \sin \Omega t + \frac{\omega_o - \omega}{\Omega} \left[\frac{2V}{\hbar \Omega} N(0) - \frac{\omega_o - \omega}{\Omega} Q(0) \right] (\cos \Omega t - 1) + Q(0) .$$

(1.106)

and

$$N'(t) = -\frac{2V P(0)}{\hbar \Omega} \sin \Omega t + \frac{2V}{\hbar \Omega} \left[\frac{2V}{\hbar \Omega} N(0) - \frac{\omega_o - \omega}{\Omega} Q(0) \right] (\cos \Omega t - 1) + N(0) \quad (1.107)$$

and

$$\Omega = \sqrt{(\omega_o - \omega)^2 + \left(\frac{2V}{\hbar} \right)^2} .$$

(1.108)

To express the solution in the lab (non-rotating frame), recall that

$$\mathbf{M}'(t) = Q'(t)\mathbf{i}_x + P'(t)\mathbf{i}_y - N'(t)\mathbf{i}_z$$

(1.109)

and

$$\mathbf{i}'_x = \cos \omega t \, \mathbf{i}_x - \sin \omega t \, \mathbf{i}_y \qquad \text{and} \qquad \mathbf{i}'_y = \sin \omega t \, \mathbf{i}_x + \cos \omega t \, \mathbf{i}_y .$$

(1.110)

Hence, the coefficients of the vectors in the stationary frame are

$$
\begin{aligned}
Q(t) &= Q'(t) \cos \omega t + P'(t) \sin \omega t & (1.111) \\
P(t) &= P'(t) \cos \omega t - Q'(t) \sin \omega t \qquad \text{and} & (1.112) \\
N'(t) &= N(t) . & (1.113)
\end{aligned}
$$

An instructive example to consider is for the state to be initially in the lower energy state, so that $N(0) = -1$, and $Q(0) = P(0) = 0$. Therefore,

$$Q'(t) = \frac{\omega_o - \omega}{\Omega} \frac{2V}{\hbar \Omega} (\cos \Omega t - 1)$$

(1.114)

and

$$P'(t) = -\frac{2V}{\hbar \Omega} \sin \Omega t .$$

(1.115)

and

$$N'(t) = - \left(\frac{2V}{\hbar \Omega} \right)^2 (\cos \Omega t - 1) - 1 .$$

(1.116)

and, consequently,

$$Q(t) = \frac{\omega_o - \omega}{\Omega} \frac{2V}{\hbar \Omega} (\cos \Omega t - 1) \cos \omega t - \frac{2V}{\hbar \Omega} \sin \Omega t \sin \omega t .$$

(1.117)

and

$$P(t) = -\frac{\omega_o - \omega}{\Omega} \frac{2V}{\hbar \Omega} (\cos \Omega t - 1) \sin \omega t - \frac{2V}{\hbar \Omega} \sin \Omega t \cos \omega t .$$

(1.118)

and

$$N(t) = 2 \left(\frac{2V}{\hbar \Omega} \right)^2 \sin^2 \Omega t/2 - 1$$

(1.119)

Figure is blank due to unavailable original.

Figure 1.5: Time average of ρ_{22} vs. driving frequency ω.

The probability of the system being in the excited state if initially in the ground state is

$$\rho_{22} = 1 - \rho_{11} = \left(\frac{2V}{\hbar\Omega}\right)^2 \sin^2 \Omega t/2 \tag{1.120}$$

$$= \frac{1}{2}\frac{(2V/\hbar)^2}{(\omega - \omega_o)^2 + (2V/\hbar)^2}\left(1 - \sin\sqrt{(\omega - \omega_o)^2 + (2V/\hbar)^2}t\right) \tag{1.121}$$

At resonance, when $\omega = \omega_o$, the two states undergo a full Rabi oscillation with frequency $2V/\hbar$. Note that in the driven case, the frequency of the oscillation on resonance is given by the strength of the potential and not the energy difference. Off resonance, the Rabi oscillation is no longer full. On average over time,

$$\langle\langle\rho_{22}(t)\rangle\rangle = \frac{1}{2}\frac{(2V/\hbar)^2}{(\omega - \omega_o)^2 + (2V/\hbar)^2} \tag{1.122}$$

which is plotted in Fig. 1.5 The line shape is Lorentzian with a full width at half maximum of $2V/\hbar$.

1.5.3   On-resonance features

Consider the on-resonance condition in the rotating frame. We have found in Eqn. 1.114—1.116 for a system that starts with $N(0) = -1$, that is, it starts fully in the lower state with $P'(0) = Q'(0) = 0$,

$$N'(t) = -\cos 2Vt/\hbar \quad\text{and}\quad P'(t) = -\sin 2Vt/\hbar \quad\text{and}\quad Q'(t) = 0\,. \tag{1.123}$$

This is exactly the same solution that was found for the time-independent solution in Eqn. 1.86. However, note that in this case that V is the amplitude of the driving sinusoidal potential; whereas, before, the solution was for a constant potential at the point where $\Delta = 0$. A similar result would hold if the solution for any arbitrary initial condition.

Hence, the unitary matrix in the rotating frame at resonance is, to within an overall phase factor, the same as in the static case at $\Delta = 0$ and is given by Eqn. 1.49 (here V is positive)

$$U'(t) = \begin{pmatrix} \cos Vt/\hbar & -i \sin Vt/\hbar \\ -i \sin Vt/\hbar & \cos Vt/\hbar \end{pmatrix} \tag{1.124}$$

Likewise, the wave functions on-resonance will also have the same form. This means, that if logical operations are consider in the rotating frame, a π-pulse can be performed by applying a frequency on resonance $\omega = \omega_o$ for a duration of $2Vt/\hbar = \pi$, so that

$$U'_\pi \begin{pmatrix} 1 \\ 0 \end{pmatrix} = -i \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{1.125}$$

and $\text{NOT} = iU_\pi$. Here the notion of a "pulse" has a clearer meaning. Similarly, an equal superposition of states can be found by performing a $\pi/2$-pulse in which a frequency on resonance $\omega = \omega_o$ is applied for a duration of $2Vt/\hbar = \pi/2$ so that

$$U'_{\pi/2} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix}. \tag{1.126}$$

The resulting state is $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}$.

1.5.4 Time dependent wave functions and unitary evolution matrix

The procedure for finding the wave function for the sinusoidal driving potential follows the same general insights of that used for the density matrix approach: The time-dependent potential problem is recast into a time-independent problem by going to the rotating frame of reference. However, we will not carry out the algebra for this problem but only state the results, and outline the approach is given in the problems.

We denote the wave function as a linear combination of basis states

$$\psi(t) = c_1(t)\phi_1 + c_2(t)\phi_2 \tag{1.127}$$

and the time dependence of the coefficients is given by Eqn. 1.88

$$i\hbar \frac{d}{dt} \begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix} = \begin{pmatrix} \bar{E} - \Delta & Ve^{i\omega t} \\ V^* e^{-i\omega t} & \bar{E} + \Delta \end{pmatrix} \begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix} \tag{1.128}$$

where V is a real constant.

If the initial wave function is $\psi(0) = \phi_1$, so that $c_1^a(0) = 1$ and $c_2^a(0) = 0$, then the state which we label a evolves such that

$$c_1^a(t) = e^{-i\bar{E}t/\hbar} e^{i\frac{\omega}{2}t} \left[\cos \frac{\Omega t}{2} + i \frac{\omega_o - \omega}{\Omega} \sin \frac{\Omega t}{2} \right] \tag{1.129}$$

$$c_2^a(t) = -ie^{-i\bar{E}t/\hbar} e^{-i\frac{\omega}{2}t} \frac{2V}{\hbar\Omega} \sin \frac{\Omega t}{2} \tag{1.130}$$

where as above $\omega_o = 2\Delta/2$ and $\Omega = \sqrt{(\omega_o - \omega)^2 + (2V/\hbar)^2}$. Likewise, if the initial wave function is $\psi(0) = \phi_2$, so that $c_2^b(0) = 1$ and $c_1^b(0) = 0$, then the state which we label b

evolves such that

$$c_2^b(t) \;=\; e^{-i\bar{E}t/\hbar} e^{-i\frac{\omega}{2}t}\left[\cos\frac{\Omega t}{2} - i\frac{\omega_o - \omega}{\Omega}\sin\frac{\Omega t}{2}\right] \tag{1.131}$$

$$c_1^b(t) \;=\; -ie^{-i\bar{E}t/\hbar} e^{i\frac{\omega}{2}t}\frac{2V}{\hbar\Omega}\sin\frac{\Omega t}{2}\,. \tag{1.132}$$

For any arbitrary initial state give by $\psi(0) = a\phi_1 + b\phi_2$, then

$$\psi(t) = \left[ac_1^a(t) + bc_1^b(t)\right]\phi_1 + \left[bc_2^b(t) + ac_2^a(t)\right]\phi_2\,. \tag{1.133}$$

Equivalently, the unitary evolution operator is given by

$$U(t) = e^{-i\bar{E}t/\hbar}\begin{pmatrix} e^{i\frac{\omega}{2}t}\left[\cos\frac{\Omega t}{2} + i\frac{\omega_o - \omega}{\Omega}\sin\frac{\Omega t}{2}\right] & -ie^{i\frac{\omega}{2}t}\frac{2V}{\hbar\Omega}\sin\frac{\Omega t}{2} \\ -ie^{-i\frac{\omega}{2}t}\frac{2V}{\hbar\Omega}\sin\frac{\Omega t}{2} & e^{-i\frac{\omega}{2}t}\left[\cos\frac{\Omega t}{2} - i\frac{\omega_o - \omega}{\Omega}\sin\frac{\Omega t}{2}\right]\end{pmatrix}\,. \tag{1.134}$$

At resonance, the unitary evolution matrix is given by

$$U_{\omega=\omega_0}(t) = e^{-i\bar{E}t/\hbar}\begin{pmatrix} e^{i\frac{\omega}{2}t}\cos Vt/\hbar & -ie^{i\frac{\omega}{2}t}\sin Vt/\hbar \\ -ie^{-i\frac{\omega}{2}t}\sin Vt/\hbar & e^{-i\frac{\omega}{2}t}\cos Vt/\hbar\end{pmatrix} \tag{1.135}$$

At time $t = 0$ the unitary evolution matrices and $U'(t)$ (Eqn. 1.124) in the rotating frame and $U_{\omega=\omega_0}(t)$ in the laboratory frame are the same since the two coordinate systems coincide then. The overall phase factor of $e^{-i\bar{E}t/\hbar}$ does not change the physics of the states. But for other times, the additional phase factors of $e^{\pm i\frac{\omega}{2}t}$ account for the difference between the two systems at resonance.

1.6   The ideal two state system: Spin 1/2 particles

Particles which have a magnetic moment μ have an energy in a magnetic field given by

$$H_{\text{spin}} = -\vec{\mu}\cdot\mathbf{B} \tag{1.136}$$

The magnetic moment is given by $\mu = ge\hbar/4m$ where m is the mass of the particle and g is known as the g=factor and $g = 2$ for the proton and neutron and $g = -2$ for the electron.

Particles, such as electrons, protons, and neutrons, are fermions and are distinguished by having a two-state quantum mechanical label called spin. These two states can be represented by by the two-state systems that we have been studying, and will be denoted here by a column vector. Quantum mechanically it is observed that the vector magnetic moment operator of this two-state system is given by

$$\vec{\mu} = \frac{ge\hbar}{4m}\left[\hat{\sigma}_x\mathbf{i}_x + \hat{\sigma}_y\mathbf{i}_y + \hat{\sigma}_z\mathbf{i}_z\right] \tag{1.137}$$

where the σ's are know as the Pauli matrices

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{1.138}$$

The Pauli matrices have the interesting properties that $\hat{\sigma}_x\hat{\sigma}_y = i\hat{\sigma}_z$ and for all cyclical permutations. Also $\hat{\sigma}_j^2 = 1$. And any two dimensional matrix can be represented by a linear combination of Pauli matrices and the identity matrix.

Hamiltonian is then given by

$$H_{\text{spin}} = -\mu\left[\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}B_x + \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}B_y + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}B_z\right] \tag{1.139}$$

For the rest of the discussion, we consider the proton where μ is positive. If $B = B_z i_z$ and B_z is independent of time, then

$$H_{\text{spin}} = \mu\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}B_z \tag{1.140}$$

and the eigen vectors are denoted are the two states denoted as spin up and spin down and given by

$$|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \text{and} \qquad |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{1.141}$$

with energies $-\mu B_x$ and $+\mu B_x$ respectively. If an additional time-dependent field in the xy-plane is applied such that

$$\mathbf{B}(t) = -b\left(\cos\omega t \mathbf{i}_x - \sin\omega t \mathbf{i}_y\right) + B_z\mathbf{i}_z. \tag{1.142}$$

Therefore, the Hamiltonian is

$$H_{\text{spin}} = \begin{pmatrix} -\mu B_z & \mu b e^{i\omega t} \\ \mu b e^{-i\omega t} & \mu B_z \end{pmatrix} \tag{1.143}$$

This Hamiltonian is of the same form that was discussed for a sinusoidal potential drive, Here $V = \mu b$ and $\hbar\omega_o = 2\Delta = 2\mu B_z$.

In the general state,

$$\langle \vec{\mu} \rangle = \text{tr}\left(\hat{\rho}\vec{\mu}\right) \tag{1.144}$$

and we find that

$$\langle \vec{\mu}_x \rangle = \mu Q(t) \qquad \langle \vec{\mu}_y \rangle = \mu P(t) \qquad \text{and} \qquad \langle \vec{\mu}_z \rangle = -\mu N(t). \tag{1.145}$$

Therefore, the dynamics of the spin system is the same as that of the two level system. Here the strength of the parameters are controlled by the magnetic field. For example, the z-component of the magnetic field determines the energy difference $\Delta = 2\mu B_z$. Transitions from one state to the other can then be done by driving the system on resonance, that is, by putting an oscillating magnetic field in the xy-plane with a frequency equal to the energy difference. This is the principle of Nuclear Magnetic Resonance, where the field is of the order of a few tesla and the characteristic frequency is in the radio frequency regime. Hence, by putting a human subject in the core of a large magnet and then applying a magnetic field tuned to the energy difference of hydrogen nuclei (protons) in water molecules, one can absorb more energy the greater the concentration of water. Since different tissues have different concentrations, the tissues can be imaged. In organic molecules, the frequency of the energy difference is changed by the proximity of other atomics in the vicinity of the hydrogen nuclei. In this way, different neighbors can be determined. Furthermore, by adjusting the time of application of this oscillating magnetic field, one can cause the system to go from one state to the other, and hence do a π-pulse for quantum logic operations.

Chapter 2

3D Rotation Matrices for the Two-State System

2.1 σ_z Drive: Density Matrix Approach

2.1.1 General formulation

The general two-state Hamiltonian is written as

$$\hat{H} = \begin{pmatrix} \bar{E} - \Delta & V \\ V^* & \bar{E} + \Delta \end{pmatrix} \tag{2.1}$$

The density matrix can be written in terms of three quantities

$$N(t) = \rho_{22} - \rho_{11} \tag{2.2}$$

and

$$Q(t) = \rho_{21} + \rho_{12} \tag{2.3}$$

and

$$P(t) = \frac{1}{i}(\rho_{21} - \rho_{12}). \tag{2.4}$$

So that the time evolution is given by the Bloch equations,

$$\frac{d}{dt}\hat{\rho} = -\frac{1}{i\hbar}\left[\hat{\rho}, \hat{H}\right]. \tag{2.5}$$

which results in

$$\frac{d}{dt}N(t) = -\frac{1}{i\hbar}\left\{Q(t)(V - V^*) + iP(t)(V + V^*)\right\} \tag{2.6}$$

and

$$\frac{d}{dt}Q(t) = \frac{2\Delta}{\hbar}P(t) + \frac{1}{i\hbar}N(t)(V - V^*) \tag{2.7}$$

and

$$\frac{d}{dt}P(t) = -\frac{2\Delta}{\hbar}Q(t) + \frac{1}{\hbar}N(t)(V + V^*) \tag{2.8}$$

2.1.2 Method of Solution: Effective Fields in Lab frame

The above equations can be recast into an equivalent algebraic problem of a magnetic moment of magnetization $\mathbf{M}$ in a magnetic field $\mathbf{B}$.

The density matrix can be written as

$$\rho = \begin{pmatrix} \frac{1+M_z}{2} & \frac{M_x - iM_y}{2} \\ \frac{M_x + iM_y}{2} & \frac{1-M_z}{2} \end{pmatrix} \tag{2.9}$$

and the Hamiltonian as

$$\hat{H} = \bar{E}I + \begin{pmatrix} \frac{H_z}{2} & \frac{H_x - iH_y}{2} \\ \frac{H_x + iH_y}{2} & \frac{-H_z}{2} \end{pmatrix} \tag{2.10}$$

This allows the identification

$$
\begin{aligned}
M_x = Q(t) &= \rho_{21} + \rho_{12} & (2.11) \\
M_y = P(t) &= \frac{1}{i}(\rho_{21} - \rho_{12}) & \\
M_z = -N(t) &= \rho_{11} - \rho_{22} &
\end{aligned}
$$

and

$$
\begin{aligned}
H_x &= V + V^* & (2.12) \\
H_y &= V - V^* & \\
H_z &= -2\Delta &
\end{aligned}
$$

The time dependence of the density matrix is

$$\frac{d}{dt}\hat{\rho} = -\frac{1}{i\hbar}\left[\hat{\rho}, \hat{H}\right] . \tag{2.13}$$

then becomes

$$
\begin{pmatrix} \frac{d}{dt}M_z & \frac{d}{dt}(M_x - iM_y) \\ \frac{d}{dt}(M_x + iM_y) & \frac{d}{dt}M_z \end{pmatrix}
$$
$$= \frac{-1}{\hbar}\begin{pmatrix} i(M_xH_y - M_yH_x) & i(M_yH_z - M_zH_y) + (M_zH_x - M_xH_z) \\ i(M_yH_z - M_zH_y) - (M_zH_x - M_xH_z) & -i(M_xH_y - M_yH_x) \end{pmatrix} \tag{2.14}$$

This is equivalent to

$$\frac{d}{dt}\mathbf{M}(t) = \mathbf{M}(t) \times \gamma\mathbf{B}(t) , \tag{2.15}$$

where $\gamma = 1/\hbar$ and

$$\mathbf{B} = -\mathbf{H} \tag{2.16}$$

and

$$\mathbf{M}(t) = M_x\mathbf{i}_x + M_y\mathbf{i}_y + M_z\mathbf{i}_z \tag{2.17}$$

and

$$\mathbf{H}(t) = H_x\mathbf{i}_x + H_y\mathbf{i}_y + H_z\mathbf{i}_z . \tag{2.18}$$

The problem then maps on to a Magnetization in a magnetic field such that the Hamiltonian is (with $\bar{E} = 0$),

$$\hat{H} = -\gamma\hat{\mathbf{I}} \cdot \mathbf{B} \tag{2.19}$$

where $\mathbf{I} = \mathbf{I_x i_x} + \mathbf{I_y i_y} + \mathbf{I_z i_z}$. is the spin vector with $I_i = \sigma_i/2$.

To understand the dynamics of the system, we solve the equivalent Bloch Equations of Eqn. 2.15 in the simple case of a constant field along the z direction; $\mathbf{B} = B_z \mathbf{i}_z$. From Eqn. 2.15

$$\frac{d}{dt} M_x = \gamma M_y B_z \qquad (2.20)$$

$$\frac{d}{dt} M_y = -\gamma M_x B_z$$

which leads to the solutions with initial values

$$M_x(t) = M_x(0) \cos \gamma B_z t + M_y(0) \sin \gamma B_z t \qquad (2.21)$$
$$M_y(t) = M_y(0) \cos \gamma B_z t - M_x(0) \sin \gamma B_z t \,.$$

We will also adopt the sign convention that $\omega_o = -\gamma B_z$ so that with $\gamma = 1/\hbar$, a magnetization vector in a z-directed field rotates in the counter-clockwise direction (right-hand rule) with frequency ω_o. Note that is means that it rotates in the clock-wise direction with frequency γB_z. Hence,

$$M_x(t) = M_x(0) \cos \omega_o t - M_y(0) \sin \omega_o t \qquad (2.22)$$
$$M_y(t) = M_y(0) \cos \omega_o t + M_x(0) \sin \omega_o t \,.$$

We can write this as

$$\begin{pmatrix} M_x(t) \\ M_y(t) \\ M_z(t) \end{pmatrix} = \begin{pmatrix} \cos \omega_o t & -\sin \omega_o t & 0 \\ \sin \omega_o t & \cos \omega_o t & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} M_x(0) \\ M_y(0) \\ M_z(0) \end{pmatrix} \qquad (2.23)$$

The rotation of a vector about the z-axis by an angle ϕ is given by the rotation matrix

$$R_z(\phi) = \begin{pmatrix} \cos \phi & -\sin \phi & 0 \\ \sin \phi & \cos \phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad (2.24)$$

Therefore, for a constant field along the z-axis, the magnetization precesses (rotates) about the z-axis with angle $\omega_o t$ where $\omega_o = -\gamma B_z$,

$$\mathbf{M}(t) = R_z(\omega_o t) \mathbf{M}(0) \qquad (2.25)$$

The adoption of the minus sign in ω is useful since it makes a positive field along z cause a positive rotation about z in mathematical terms, but remember that rotation angle happens to be negative. There are many conventions on how to handle this minus sign, and this is the one we will use in this class (see Spin Dynamics, by M. H. Levitt).

Often one want to know how the magnetization at time t_1 evolves up to time t_2 during the interval $\tau = t_2 - t_1$. From a shift in the time axis, one finds

$$\mathbf{M}(t_2) = R_z(\omega_o \tau) \mathbf{M}(t_1) \qquad (2.26)$$

Figure is blank due to unavailable original.

Figure 2.1: A rotating reference frame, which is taken to be along the z-axis here. The rotation frequency it ω_{ref} and the initial offset angle is ϕ_{ref}. The full angle of rotation is $\Phi(t) = \omega_{\mathrm{ref}} t + \phi_{\mathrm{ref}}$.

Let's consider some initial conditions which are valuable in quantum computing. First consider the case where the initial condition is $\mathbf{M}(0) = M_z(0)\mathbf{i}_z$. This implies that initial quantum state is (to within an irrelevant phase factor), $\psi(0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$. This state evolves as $\mathbf{M}(t) = R_z(\omega_o t)\mathbf{M}(0) = M_z\mathbf{i}_z$. Hence, the state remain the same (to within a phase factor). The projection of $\mathbf{M}(t)$ along the z-axis, which is the axis of quantization, remains the same and is equal to one.

Secondly, consider the initial condition of $\mathbf{M}(0) = \mathbf{i}_x$ so that the initial magnetization is along the x-axis. This corresponds to the initial quantum state $\psi(0) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ which is an eigen state of the σ_x operator. The projection of this state along the z-axis is zero, meaning that it is as equally likely for this state to be in the spin-up state as the spin-down state. The field in the z direction causes the magnetization to rotate with about the z-axis, in the xy-plane with a constant frequency ω_o. We take $B_z \geq 0$, so that $\omega_o \leq 0$. So after a time $\tau_{\pi/2} = \pi/(-2\omega_o)$, the magnetization vector is along the $-y$-axis and the state is then an eigen state of the σ_y operator. The state after this $-\pi/2$-rotation is, to within a phase factor, $\psi(t_{\pi/2}) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}$. Likewise, after a time, $\tau_\pi = \pi/(-\omega_o)$, the magnetization is along the $-x$-axis, so that the state has been transformed to the spin-down state along the x-axis. This corresponds to the state, $\psi(0) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$.

2.1.3   Effective Fields in a Rotating Frame

In finding the effects of an ac driving field on the qubit, it will be convenient to study the dynamics in a rotating frame. Consider the rotating frame which rotates with a constant angular velocity ω_{ref} about a given given axis denoted by the vector $\vec{\omega}_{\mathrm{ref}}$ as shown in Figure 2.1. The initial offset angle is ϕ_{ref}. The full angle of rotation is $\Phi(t) = \omega_{\mathrm{ref}} t + \phi_{\mathrm{ref}}$.

The same physical vector is denoted by $\mathbf{A}(t)$ in the stationary frame and by $\tilde{\mathbf{A}}(t)$ in the rotating frame. We write the same physical vector in each of the two reference frames as

$$\mathbf{A}(t) = A_x \mathbf{i}_x + A_y \mathbf{i}_y + A_z \mathbf{i}_z \tag{2.27}$$

and

$$\tilde{\mathbf{A}}(t) = \tilde{A}_x \tilde{\mathbf{i}}_x + \tilde{A}_y \tilde{\mathbf{i}}_y + \tilde{A}_z \tilde{\mathbf{i}}_z \tag{2.28}$$

We can related the coefficients in each frame by $\tilde{\mathbf{A}}(t) = R_{\text{ref}}(-\Phi(t))\mathbf{A}(t)$, where the subscript on the rotation matrix denotes the direction of the rotation axis.

The unit vectors in the rotating frame change with time by

$$\frac{d}{dt}\tilde{\mathbf{i}}_x = \vec{\omega}_{\text{ref}} \times \mathbf{i}_x \quad \text{and} \quad \frac{d}{dt}\tilde{\mathbf{i}}_y = \vec{\omega}_{\text{ref}} \times \mathbf{i}_y \quad \text{and} \quad \frac{d}{dt}\tilde{\mathbf{i}}_z = \vec{\omega}_{\text{ref}} \times \mathbf{i}_z \,. \tag{2.29}$$

The time rate of change of the physical vector is then given by

$$\begin{aligned}
\frac{d}{dt}\mathbf{A}(t) &= \frac{dA_x}{dt}\mathbf{i}_x + \frac{dA_y}{dt}\mathbf{i}_y + \frac{dA_z}{dt}\mathbf{i}_z \\
&= \frac{\partial \tilde{A}_x}{\partial t}\tilde{\mathbf{i}}_x + \frac{\partial \tilde{A}_y}{\partial t}\tilde{\mathbf{i}}_y + \frac{\partial \tilde{A}_z}{\partial t}\tilde{\mathbf{i}}_z + \tilde{A}_x \frac{d\tilde{\mathbf{i}}_x}{dt} + \tilde{A}_y \frac{d\tilde{\mathbf{i}}_y}{dt} \tilde{A}_z \frac{d\tilde{\mathbf{i}}_z}{dt} \\
&= \frac{d}{dt}\tilde{\mathbf{A}}(t)
\end{aligned} \tag{2.30}$$

where $\frac{\partial A_x}{\partial t}$ denotes the partial time derivative. The above equation can be written compactly as

$$\frac{d}{dt}\mathbf{A}(t) = \frac{\partial}{\partial t}\tilde{\mathbf{A}} + \vec{\omega}_{\text{ref}} \times \tilde{\mathbf{A}} \tag{2.31}$$

Here $\partial \tilde{\mathbf{A}}(t)/\partial t$ is the time rate of change of the vector as seen by an observer in the rotating reference frame.

The Bloch equations of motion can now be expressed in the rotating frame. In the stationary frame

$$\frac{d}{dt}\mathbf{M}(t) = \mathbf{M}(t) \times \gamma \mathbf{B}(t) \tag{2.32}$$

or equivalently expressed with the vectors in the rotating frame

$$\frac{d}{dt}\tilde{\mathbf{M}}(t) = \tilde{\mathbf{M}}(t) \times \gamma \tilde{\mathbf{B}}(t) \,. \tag{2.33}$$

Using the above we can write the Bloch equations as

$$\frac{\partial}{\partial t}\tilde{\mathbf{M}} + \vec{\omega}_{\text{ref}} \times \tilde{\mathbf{M}} = \tilde{\mathbf{M}}(t) \times \gamma \tilde{\mathbf{B}}(t) \,. \tag{2.34}$$

Equivalently,

$$\frac{\partial}{\partial t}\tilde{\mathbf{M}}(t) = \tilde{\mathbf{M}}(t) \times \gamma \tilde{\mathbf{B}}_{\text{eff}}(t) \tag{2.35}$$

where

$$\tilde{\mathbf{B}}_{\text{eff}}(t) = \mathbf{B}(t) + \frac{\vec{\omega}}{\gamma} \,. \tag{2.36}$$

Hence, in terms of the time derivative of the magnetization vector in the rotating frame, the Bloch equations are of the same form as in the stationary frame, but with an additional magnetic field along the direction of rotation.

The initial reference angle ϕ_{ref} does not enter into the equations of motion directly, but only through the initial conditions. By convention,

$$
\begin{aligned}
\phi_{\text{ref}} &= \pi & \text{if} \quad \gamma > 0 \\
\phi_{\text{ref}} &= 0 & \text{if} \quad \gamma < 0
\end{aligned}
\tag{2.37}
$$

Since $\gamma = 1/\hbar$ we will take $\phi_{\text{ref}} = \pi$

2.2   Problems

Problem 1 *Wave functions the sinusoidal drive.*

Denote the wave function as a linear combination of basis states

$$
\psi(t) = c_1(t)\phi_1 + c_2(t)\phi_2
\tag{2.38}
$$

and the time dependence of the coefficients is given by Eqn. 1.128 for a sinusoidal driving potential of $V(t) = Ve^{i\omega t}$ is

$$
i\hbar \frac{d}{dt} \begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix} = \begin{pmatrix} \bar{E} - \Delta & Ve^{i\omega t} \\ V^* e^{-i\omega t} & \bar{E} + \Delta \end{pmatrix} \begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix}
\tag{2.39}
$$

where V is a real constant.

(a) Let $c_i(t) = b_i(t)e^{-i\bar{E}t/hbar}$ and show that

$$
i\hbar \frac{d}{dt} \begin{pmatrix} b_1(t) \\ b_2(t) \end{pmatrix} = \begin{pmatrix} -\Delta & Ve^{i\omega t} \\ V^* e^{-i\omega t} & \Delta \end{pmatrix} \begin{pmatrix} b_1(t) \\ b_2(t) \end{pmatrix}
\tag{2.40}
$$

(b) Now let $b_1(t) = b_1 e^{i\lambda_1 t/hbar}$ and $b_2(t) = b_2 e^{i\lambda_2 t/hbar}$ where b_1 and b_2 are independent of time. Show that if $\lambda_1 = \lambda_2 \pm \hbar\omega$, then the resulting equations are and eigen value problem which independent of time.

(c) Find the resulting eigen values, and show that there are two values each λ_i which can be written as $\lambda_{1,\pm} = \hbar(\omega \pm \Omega)/2$ and $\lambda_{2,\pm} = \hbar(-\omega \pm \Omega)/2$ where $\Omega = \sqrt{(\omega_o - \omega)^2 + (2V/\hbar)^2}$.

(d) Write the form of the general solution for in terms of these four eigen values. Use this and match initial conditions to find $c_1^a(t)$, $c_2^a(t)$, $c_1^b(t)$, and $c_2^b(t)$ as in Eqns. 1.132 and **??**.

(e) Show that the Unitary evolution matrix of Eqn. 1.135 is given by

$$
\begin{pmatrix} c_1^a(t) & c_2^a(t) \\ c_2^a(t) & c_2^b(t) \end{pmatrix}
\tag{2.41}
$$