Problem 1: Spin-1/2 particle in a magnetic field

Let us consider a spin-1/2 particle in a magnetic field directed along the axis of quantization, $\boldsymbol{B} = B\boldsymbol{z}$. The Hamiltonian is given by

$$\hat{H} = \frac{\hbar\omega}{2}\sigma_z = \frac{\hbar\omega}{2}\left(|0\rangle\langle 0| - |1\rangle\langle 1|\right) \tag{1}$$

where ω is the Larmor frequency which is proportional to B. There is actually a negative sign up front, but it is usually absorbed into ω. The particle is not necessarily in a pure state, so it is described by a density matrix

$$\rho = \frac{1}{2}(1 + \boldsymbol{r}\cdot\boldsymbol{\sigma}) = \sum_{i,j}\rho_{ij}\,|i\rangle\langle j| \tag{2}$$

We want to calculate the time evolution of the density matrix using the equation of motion

$$i\hbar\dot{\rho} = \left[\hat{H}, \rho\right] \tag{3}$$

Let us go through two different methods to solve this problem.

Method 1: Using the sigma matrices

The commutation relation for sigma matrices comes in handy here:

$$\left[\sigma_i, \sigma_j\right] = 2i\varepsilon_{ijk}\sigma_k \tag{4}$$

We compute the commutation relation:

$$\begin{aligned}\left[\hat{H}, \rho\right] &= \frac{\hbar\omega}{4}[\sigma_z, 1 + \boldsymbol{r}\cdot\boldsymbol{\sigma}] \\ &= \frac{i\hbar\omega}{2}\left(-x\sigma_y + y\sigma_x\right) \\ &= \frac{i\hbar\omega}{2}\begin{pmatrix} 0 & ix+y \\ -ix+y & 0\end{pmatrix}\end{aligned} \tag{5}$$

Next, we can write

$$\rho = \frac{1}{2}\begin{pmatrix} 1+z & x-iy \\ x+iy & 1-z\end{pmatrix} \tag{6}$$

so that

$$\dot{\rho} = \frac{1}{2}\begin{pmatrix} \dot{z} & \dot{x}-i\dot{y} \\ \dot{x}+i\dot{y} & -\dot{z}\end{pmatrix} \tag{7}$$

Putting these results into (3), we have

$$\begin{aligned} i\hbar\frac{1}{2}\begin{pmatrix} \dot{z} & \dot{x}-i\dot{y} \\ \dot{x}+i\dot{y} & -\dot{z}\end{pmatrix} &= \frac{i\hbar\omega}{2}\begin{pmatrix} 0 & ix+y \\ -ix+y & 0\end{pmatrix} \\ \begin{pmatrix} \dot{z} & \dot{x}-i\dot{y} \\ \dot{x}+i\dot{y} & -\dot{z}\end{pmatrix} &= \omega\begin{pmatrix} 0 & ix+y \\ -ix+y & 0\end{pmatrix}\end{aligned} \tag{8}$$

We obtain three equations:

$$\begin{aligned}\dot{x} &= \omega y \\ \dot{y} &= -\omega x \\ \dot{z} &= 0\end{aligned} \tag{9}$$

The solutions are

$$\begin{aligned} x(t) &= A\cos(\omega t) + B\sin(\omega t) \\ y(t) &= A\cos(\omega t) - B\sin(\omega t) \\ z(t) &= const.\end{aligned} \tag{10}$$

In the Bloch sphere representation, the density matrix vector rotates about the positive z-axis.

Method 2: Expanding the density matrix

We have

$$
\begin{aligned}
\frac{2}{\hbar\omega}\left[\hat{H},\rho\right] &= \left[|0\rangle\langle 0| - |1\rangle\langle 1|\right]\left[\sum_{i,j}\rho_{ij}|i\rangle\langle j|\right] - \left[\sum_{i,j}\rho_{ij}|i\rangle\langle j|\right]\left[|0\rangle\langle 0| - |1\rangle\langle 1|\right] \\
&= \sum_{i,j}\rho_{ij}|0\rangle\langle 0|i\rangle\langle j| - \sum_{i,j}\rho_{ij}|1\rangle\langle 1|i\rangle\langle j| - \sum_{i,j}\rho_{ij}|i\rangle\langle j|0\rangle\langle 0| + \sum_{i,j}\rho_{ij}|i\rangle\langle j|1\rangle\langle 1| \\
&= \sum_{j}\rho_{0j}|0\rangle\langle j| - \sum_{j}\rho_{1j}|1\rangle\langle j| - \sum_{i}\rho_{i0}|i\rangle\langle 0| + \sum_{i}\rho_{i1}|i\rangle\langle 1| \\
&= 2\rho_{01}|0\rangle\langle 1| - 2\rho_{10}|1\rangle|0\rangle \\
&= 2\begin{pmatrix} 0 & \rho_{01} \\ -\rho_{10} & 0 \end{pmatrix}
\end{aligned} \tag{11}
$$

Putting this into (3), we have

$$
i\hbar\begin{pmatrix} \dot{\rho}_{00} & \dot{\rho}_{01} \\ \dot{\rho}_{10} & \dot{\rho}_{11} \end{pmatrix} = \hbar\omega\begin{pmatrix} 0 & \rho_{01} \\ -\rho_{10} & 0 \end{pmatrix} \tag{12}
$$

We obtain 4 equations whose solutions are

$$
\begin{aligned}
\rho_{00}(t) &= \rho_{00}(0) \\
\rho_{01}(t) &= \rho_{01}(0)e^{-i\omega t} \\
\rho_{10}(t) &= \rho_{10}(0)e^{i\omega t} \\
\rho_{11}(t) &= \rho_{11}(0)
\end{aligned} \tag{13}
$$

Problem 2: The Rabi oscillation

We are working with a two-level system whose Hamiltonian is given by

$$
\begin{aligned}
\hat{H} &= \frac{\Delta}{2}\sigma_z + \Omega\delta_x \\
&= \frac{\Delta}{2}|0\rangle\langle 0| - \frac{\Delta}{2}|1\rangle\langle 1| + \Omega|0\rangle\langle 1| + \Omega|1\rangle\langle 0| \\
&= \begin{pmatrix} \frac{\Delta}{2} & \Omega \\ \Omega & \frac{-\Delta}{2} \end{pmatrix}
\end{aligned} \tag{14}
$$

Let

$$
\rho = \begin{pmatrix} a & b \\ b^* & c \end{pmatrix} \tag{15}
$$

Then,

$$
\left[\hat{H},\rho\right] = \begin{pmatrix} \Omega\left(b^* - b\right) & \Omega(c-a) + \Delta b \\ \Omega(a-c) - \Delta b^* & \Omega\left(b - b^*\right) \end{pmatrix} \tag{16}
$$

The equation of motion can then be written as (with $\hbar = 1$)

$$
\dot{a} = i\Omega\left(b - b^*\right) \tag{17}
$$

$$
\dot{b} = i\Omega(a-c) - i\Delta b \tag{18}
$$

$$
\dot{b}^* = i\Omega(c-a) + i\Delta b^* \tag{19}
$$

$$
\dot{c} = i\Omega\left(b^* - b\right) \tag{20}
$$

Taking the complex conjugate of (18) and comparing it to (19), we can see that

$$
\begin{aligned}
c^* - a^* &= c - a \\
c^* - c &= a^* - a
\end{aligned} \tag{21}
$$

which tells us that a and c have the same imaginary parts. Actually, their imaginary parts are zero since the diagonal entries of a density matrix must be real. (18) and (19) are redundant; we only need one of them. Next, let us take the derivative of (18) with respect to time to obtain

$$\ddot{b} = i\Omega\left(\dot{a} - \dot{c}\right) - i\Delta\dot{b} \tag{22}$$

We can put in (17) and (20) to obtain

$$\ddot{b} = -2\Omega^2\left(b - b^*\right) - i\Delta\dot{b} \tag{23}$$

Using

$$\mathrm{Im}(z) = \frac{i}{2}\left(z^* - z\right) \tag{24}$$

and writing

$$b \equiv p + iq \tag{25}$$

we can separate (23) into real and imaginary parts:

$$\ddot{p} = \Delta\dot{q} \tag{26}$$

$$\ddot{q} = -4\Omega^2 q - \Delta\dot{p} \tag{27}$$

From (26), we may write

$$\dot{p} = \Delta q + C \tag{28}$$

where C is a constant. Putting this into (27), we obtain

$$\ddot{q} + \left(4\Omega^2 + \Delta^2\right)q + C\Delta = 0 \tag{29}$$

The solution to this ODE is

$$q = A\cos\left(\omega_1 t\right) + B\sin\left(\omega_1 t\right) - C\frac{\Delta}{\omega_1^2}; \qquad \omega_1^2 \equiv 4\Omega^2 + \Delta^2 \tag{30}$$

Note that the arbitrary constants corresponding to the ODE (29) are A and B; the constant C comes from (28). Putting (30) into (28), we have

$$\begin{aligned}\dot{p} &= \Delta\left(A\cos\left(\omega_1 t\right) + B\sin\left(\omega_1 t\right) - C\frac{\Delta}{\omega_1^2}\right) + C\\ p &= A\frac{\Delta}{\omega_1}\sin\left(\omega_1 t\right) - B\frac{\Delta}{\omega_1}\cos\left(\omega_1 t\right) + C\frac{4\Omega^2}{\omega_1^2}t + D\end{aligned} \tag{31}$$

With (30) and (31) we obtain

$$\begin{aligned}b &= A\frac{\Delta}{\omega_1}\sin\left(\omega_1 t\right) - B\frac{\Delta}{\omega_1}\cos\left(\omega_1 t\right) + C\frac{4\Omega^2}{\omega_1^2}t + D + i\left[A\cos\left(\omega_1 t\right) + B\sin\left(\omega_1 t\right) - C\frac{\Delta}{\omega_1^2}\right]\\ &= \left[A\frac{\Delta}{\omega_1} + iB\right]\sin\left(\omega_1 t\right) + \left[-B\frac{\Delta}{\omega_1} + iA\right]\cos\left(\omega_1 t\right) + C\frac{4\Omega^2}{\omega_1^2}t - iC\frac{\Delta}{\omega_1^2} + D\end{aligned} \tag{32}$$

Taking the complex conjugate, we have

$$b^* = \left[A\frac{\Delta}{\omega_1} - iB\right]\sin\left(\omega_1 t\right) + \left[-B\frac{\Delta}{\omega_1} - iA\right]\cos\left(\omega_1 t\right) + C\frac{4\Omega^2}{\omega_1^2}t + iC\frac{\Delta}{\omega_1^2} + D \tag{33}$$

Note that since p and q are real, so must be A, B, C, and D. Using (32) and (31) in (17) and (20), we find that

$$\begin{aligned}\dot{a} &= -2\Omega q\\ a &= -\frac{2\Omega A}{\omega_1}\sin\left(\omega_1 t\right) + \frac{2\Omega B}{\omega_1}\cos\left(\omega_1 t\right) + \frac{2C\Omega\Delta}{\omega_1^2}t + E\end{aligned} \tag{34}$$

and

$$\begin{aligned}\dot{c} &= 2\Omega q\\ c &= \frac{2\Omega A}{\omega_1}\sin\left(\omega_1 t\right) - \frac{2\Omega B}{\omega_1}\cos\left(\omega_1 t\right) - \frac{2C\Omega\Delta}{\omega_1^2}t + F\end{aligned} \tag{35}$$

where E and F are obviously real. We can interpret a and c as the probability of finding the system in the ground and excited state, respectively. But looking at 34 and 35, it seems like c goes below zero when enough time has passed. This is not true, since we have not specified the arbitrary constants yet. To see this through, let us look back at (18). The real part of the equation is given by

$$\dot{p} = \Delta q \tag{36}$$

By comparison to (28), this gives us

$$C = 0 \tag{37}$$

so our problem is solved. The next thing to do is to put in the initial condition. The Rabi oscillation starts with the particle in equilibrium with the static external field which is responsible for the term with Δz. At time $t = 0$, the perpendicular field is on and this is where the phenomenon starts. The initial equilibrium state is, of course, the ground state of the particle, and thus we may write

$$\rho(0) = |0\rangle\langle 0| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \tag{38}$$

Using (32) through (35), with $C = 0$, we obtain a set of equations:

$$-\frac{\Delta B}{\omega_1} + D + iA = 0 \tag{39}$$

$$-\frac{\Delta B}{\omega_1} + D - iA = 0 \tag{40}$$

$$\frac{2\Omega B}{\omega_1} + E = 1 \tag{41}$$

$$\frac{-2\Omega B}{\omega_1} + F = 0 \tag{42}$$

These give us

$$A = 0 \tag{43}$$

$$D = \frac{\Delta B}{\omega_1} \tag{44}$$

$$E = 1 - \frac{2\Omega B}{\omega_1} \tag{45}$$

$$F = \frac{2\Omega B}{\omega_1} \tag{46}$$

Lastly, we can once again look at (18) and evaluate the equation for $t = 0$. Since $a(0) = 1$ and $b(0) = c(0) = 0$, we obtain

$$\begin{aligned} \dot{b}(0) &= i\Omega \\ iB &= i\Omega \\ B &= \Omega \end{aligned} \tag{47}$$

The time evolution of the particle is thus given by (here the double angle identity is used)

$$\rho(t) = \begin{pmatrix} 1 - \frac{4\Omega^2}{\omega_1}\sin^2\left(\frac{\omega_1 t}{2}\right) & \frac{2\Omega\Delta}{\omega_1}\sin^2\left(\frac{\omega_1 t}{2}\right) + i\Omega\sin(\omega_1 t) \\ \frac{2\Omega\Delta}{\omega_1}\sin^2\left(\frac{\omega_1 t}{2}\right) - i\Omega\sin(\omega_1 t) & \frac{4\Omega^2}{\omega_1}\sin^2\left(\frac{\omega_1 t}{2}\right) \end{pmatrix}; \qquad \omega_1 = \sqrt{4\Omega^2 + \Delta^2} \tag{48}$$

Here is a plot showing the time evolution of each element: