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Course: **8.421 - AMO I**
Problem set: **#1**
Due: Friday, Feb 11, 2022.

1. Rabi problem.

a) The Hamitonian of the system in the Schrödinger picture is

$$\begin{aligned}\mathcal{H}_S(t) &= \hbar\begin{pmatrix}\omega_1 & \omega_R\cos\omega t\\ \omega_R\cos\omega t & \omega_2\end{pmatrix}\\ &= \frac{\hbar}{2}\begin{pmatrix}2\omega_1 & \omega_R(e^{-i\omega t}+e^{i\omega t})\\ \omega_R(e^{-i\omega t}+e^{i\omega t}) & 2\omega_2\end{pmatrix}.\end{aligned}$$

where we chosen a basis where $|1\rangle = (1\ 0)^\top$ and $|2\rangle = (0\ 1)^\top$ and used the fact that the coupling between state $|2\rangle$ and state $|1\rangle$ is $\hbar\omega_R\cos\omega t$. Let us go to rotating frame via the operator

$$T = e^{i\sigma_z\omega t/2} = \begin{pmatrix}e^{i\omega t/2} & 0\\ 0 & e^{-i\omega t/2}\end{pmatrix}$$

We have the following relations between the rest frame and rotating frame:

$$\text{States: } \left|\psi_{\text{rot}}(t)\right\rangle = T^\dagger\left|\psi(t)\right\rangle \qquad \text{Operators: } A_{\text{rot}}(t) = T^\dagger A(t)T$$

The Schrödinger equation in the rotating frame can thus be obtained from the Schrödinger equation in the rest frame. From

$$\begin{aligned}i\hbar\frac{d}{dt}\left|\psi(t)\right\rangle &= i\hbar\frac{d}{dt}\left(T\left|\psi_{\text{rot}}(t)\right\rangle\right)\\ &= i\hbar\dot{T}\left|\psi_{\text{rot}}(t)\right\rangle + i\hbar T\frac{d}{dt}\left|\psi_{\text{rot}}(t)\right\rangle\\ &= \mathcal{H}_S(t)\left|\psi\right\rangle\\ &= \mathcal{H}_S(t)T\left|\psi_{\text{rot}}(t)\right\rangle\end{aligned}$$

we deduce that $\left|\psi_{\text{rot}}(t)\right\rangle$ satisfies the equation

$$i\hbar\frac{d}{dt}\left|\psi_{\text{rot}}(t)\right\rangle = \left(T^\dagger\mathcal{H}_S(t)T - i\hbar T^\dagger\dot{T}\right)\left|\psi_{\text{rot}}(t)\right\rangle.$$

With this we may define the rotating frame Hamiltonian:

$$\mathcal{H}_{\text{rot}}(t) = T^\dagger\mathcal{H}_S(t)T - i\hbar T^\dagger\dot{T}$$

so that

$$i\hbar\frac{d}{dt}\left|\psi_{\text{rot}}(t)\right\rangle = \mathcal{H}_{\text{rot}}(t)\left|\psi_{\text{rot}}(t)\right\rangle.$$

Since both T and $\mathcal{H}_S(t)$ are given, we may compute $\mathcal{H}_{\text{rot}}(t)$ explicitly. Using Mathematica, we find

$$\mathcal{H}_{\text{rot}}(t) = \frac{\hbar}{2}\begin{pmatrix}\omega+2\omega_1 & \omega_R(1+e^{-2i\omega t})\\ \omega_R(1+e^{+2i\omega t}) & -\omega+2\omega_2\end{pmatrix}.$$

Before going any further with the calculation, we may make the **rotating wave approximation** and drop the rapidly rotating term $e^{\pm 2i\omega t}$ in the $\mathcal{H}_{\text{rot}}(t)$. Following this step, the approximate rotating frame Hamiltonian is time-independent:

$$\mathcal{H}_{\text{rot}}^{\text{RWA}} = \frac{\hbar}{2}\begin{pmatrix} \omega + 2\omega_1 & \omega_R \\ \omega_R & -\omega + 2\omega_2 \end{pmatrix}$$

Moreover, let us make the following symmetrization. Let $\omega_{\text{avg}} = (\omega_1 + \omega_2)/2$ and $\omega_0 = \omega_2 - \omega_1$, then we have

$$\mathcal{H}_{\text{rot}}^{\text{RWA}} = \frac{\hbar}{2}\begin{pmatrix} \omega + 2\omega_1 & \omega_R \\ \omega_R & -\omega + 2\omega_2 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} \omega - \omega_0 & \omega_R \\ \omega_R & -\omega + \omega_0 \end{pmatrix} + \hbar\begin{pmatrix} \omega_{\text{avg}} & 0 \\ 0 & \omega_{\text{avg}} \end{pmatrix}.$$

Let us go a step further and define the **detuning** $\delta = \omega - \omega_0$ to get

$$\mathcal{H}_{\text{rot}}^{\text{RWA}} = \frac{\hbar}{2}\begin{pmatrix} \delta & \omega_R \\ \omega_R & -\delta \end{pmatrix} + \hbar\omega_{\text{avg}}\mathbb{I}.$$

The eigenvalues of this Hamiltonian are

$$E_\pm \pm \frac{\hbar}{2}\sqrt{\delta^2 + \omega_R^2} + \hbar\omega_{\text{avg}} = \pm\frac{\hbar\Omega}{2} + \hbar\omega_{\text{avg}}$$

where we have defined the generalized Rabi frequency $\Omega_R = \sqrt{\delta^2 + \omega_R^2}$. To get eigenvectors, we solve the system

$$\mathcal{H}_{\text{rot}}^{\text{RWA}}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = E_\pm\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

under the normalization condition $|c_1|^2 + |c_2|^2 = 1$. By inspection, we must have that

$$\begin{aligned} c_2 &= \frac{E_\pm - \hbar\omega_{\text{avg}} - \hbar\delta/2}{\hbar\omega_R/2}c_1 \\ \implies &\left[1 + \left(\frac{2E_\pm}{\hbar\omega_R} - \frac{2\omega_{\text{avg}}}{\omega_R} - \frac{\delta}{\omega_R}\right)^2\right]|c_1|^2 = \left[1 + \left(\frac{\pm\sqrt{\delta^2 + \omega_R^2}}{\omega_R} - \frac{\delta}{\omega_R}\right)^2\right]|c_1|^2 = 1 \end{aligned}$$

Let us call $\cos\phi = \delta/\Omega_R$ and $\sin\phi = \omega_R/\Omega_R$. For E_+, we can simplify:

$$1 = |c_1|^2\left[1 + \left(\frac{1}{\sin\phi} - \cot\phi\right)^2\right] = \frac{1}{\cos^2(\phi/2)} \implies c_1 = \cos\frac{\phi}{2} \implies c_2 = \sin\frac{\phi}{2}.$$

We can do the same for E_- and get

$$\begin{aligned} c_1 &= +\cos\frac{\phi}{2} \implies c_2 = \sin\frac{\phi}{2} \qquad \text{for } E_+ \\ c_1 &= -\sin\frac{\phi}{2} \implies c_2 = \cos\frac{\phi}{2} \qquad \text{for } E_- \end{aligned}$$

from which we can express the eigenvectors in terms of the stationary basis vectors $|1\rangle$ and $|2\rangle$:

$$\begin{aligned} |+_{\text{rot}}(t)\rangle &= +\cos\frac{\phi}{2}|1\rangle + \sin\frac{\phi}{2}|2\rangle \\ |-_{\text{rot}}(t)\rangle &= -\sin\frac{\phi}{2}|1\rangle + \cos\frac{\phi}{2}|2\rangle \end{aligned}$$

where we have arbitrarily picked a phase to get "nice" results. This lets us write the wavefunction in the rotating frame at $t = 0$ as

$$\left|\psi_{\text{rot}}(0)\right\rangle = \left|\psi(0)\right\rangle = |1\rangle = \cos\frac{\phi}{2}\,|+_{\text{rot}}(t)\rangle - \sin\frac{\phi}{2}\,|-_{\text{rot}}(t)\rangle\,,$$

from which we can derive its time evolution (also in the rotating frame).

$$\begin{aligned}
\left|\psi_{\text{rot}}(t)\right\rangle &= e^{-i\mathcal{H}_{\text{rot}}^{\text{RWA}}t/\hbar}\left|\psi_{\text{rot}}(0)\right\rangle \\
&= \cos\frac{\phi}{2}e^{-iE_+t/\hbar}\,|+_{\text{rot}}(t)\rangle - \sin\frac{\phi}{2}e^{-iE_-t/\hbar}\,|-_{\text{rot}}(t)\rangle \\
&= e^{-i\omega_{\text{avg}}t}\left[\cos\frac{\phi}{2}e^{-i\Omega_R t/2}\,|+_{\text{rot}}(t)\rangle - \sin\frac{\phi}{2}e^{+i\Omega_R t/2}\,|-_{\text{rot}}(t)\rangle\right] \\
&= e^{-i\omega_{\text{avg}}t}\left[\cos\frac{\phi}{2}e^{-i\Omega_R t/2}\left(\cos\frac{\phi}{2}\,|1\rangle + \sin\frac{\phi}{2}\,|2\rangle\right) - \sin\frac{\phi}{2}e^{+i\Omega_R t/2}\left(-\sin\frac{\phi}{2}\,|1\rangle + \cos\frac{\phi}{2}\,|2\rangle\right)\right] \\
&= e^{-i\omega_{\text{avg}}t}\left[\left(\cos^2\frac{\phi}{2}e^{-i\Omega_R t/2} + \sin^2\frac{\phi}{2}e^{i\Omega_R t/2}\right)|1\rangle + \left(e^{-i\Omega_R t/2} - e^{i\Omega_R t/2}\right)\cos\frac{\phi}{2}\sin\frac{\phi}{2}\,|2\rangle\right] \\
&= e^{-i\omega_{\text{avg}}t}\left[\left(\cos\frac{\Omega_R t}{2} - i\cos\phi\sin\frac{\Omega_R t}{2}\right)|1\rangle - i\sin\phi\sin\frac{\Omega_R t}{2}\,|2\rangle\right] \\
&= e^{-i\omega_{\text{avg}}t}\left[\left(\cos\frac{\Omega_R t}{2} - i\frac{\delta}{\Omega_R}\sin\frac{\Omega_R t}{2}\right)|1\rangle - i\frac{\omega_R}{\Omega_R}\sin\frac{\Omega_R t}{2}\,|2\rangle\right].
\end{aligned}$$

Note that the answer above is in the rotating frame. To obtain the wavefunction in the lab frame we have to transform it back via

$$\begin{aligned}
\left|\psi(t_1)\right\rangle &= T\left|\psi_{\text{rot}}(t_1)\right\rangle \\
&= \boxed{e^{-i\omega_{\text{avg}}t}\left[e^{i\omega t/2}\left(\cos\frac{\Omega_R t}{2} - i\frac{\delta}{\Omega_R}\sin\frac{\Omega_R t}{2}\right)|1\rangle - ie^{-i\omega t/2}\frac{\omega_R}{\Omega_R}\sin\frac{\Omega_R t}{2}\,|2\rangle\right]}
\end{aligned}$$

Mathematica code:

```
(*define rest Hamiltonian*)
In[2]:= H =
h/2*{{2*w1,
wR*(E^(-I*w*t) + E^(I*w*t))}, {wR*(E^(+I*w*t) + E^(-I*w*t)),
2*w2}};

(*define T*)
In[3]:= T = MatrixExp[I*PauliMatrix[3]*w*t/2];

(*calculate rotating Hamiltonian*)
In[23]:= H1 =
FullSimplify[ConjugateTranspose[T] . H . T,
Assumptions -> {w > 0, t > 0}];

In[24]:= H2 =
FullSimplify[-I*h*ConjugateTranspose[T] . D[T, t],
Assumptions -> {w > 0, t > 0}];

(*Hrot, with RWA*)
In[22]:= Hrot = H1 + H2 /. {t -> 0}

Out[22]= {{(h w)/2 + h w1, h wR}, {h wR, -((h w)/2) + h w2}}
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b) The probability of finding the system in state $|2\rangle$ at time t_1 is

$$\boxed{P_2(t_1) = \left|\left\langle 2\middle|\psi_{\text{rot}}(t_1)\right\rangle\right|^2 = \frac{\omega_R^2}{\Omega_R^2}\sin^2\left(\frac{\Omega_R t}{2}\right)}$$

c) To do this problem, we first have to go back to the rest frame:

$$\left|\psi(t)\right\rangle = e^{-i\omega_{\text{avg}}t}\left[e^{i\omega t/2}\left(\cos\frac{\Omega_R t}{2} - i\frac{\delta}{\Omega_R}\sin\frac{\Omega_R t}{2}\right)|1\rangle - ie^{-i\omega t/2}\frac{\omega_R}{\Omega_R}\sin\frac{\Omega_R t}{2}|2\rangle\right].$$

The field is turned off, so the system evolves under the field-free time-independent Hamiltonian

$$\mathcal{H}_{\text{free}} = \hbar\begin{pmatrix}\omega_1 & 0\\ 0 & \omega_2\end{pmatrix}.$$

It is clear that with the associated unitary time evolution operator

$$U(t) = e^{-i\mathcal{H}_{\text{free}}t/\hbar}$$

we have, for $t > t_1$,

$$\boxed{\left|\psi(t > t_1)\right\rangle = e^{-i\omega_{\text{avg}}t}\left[e^{-i\omega_1 t}e^{i\omega t/2}\left(\cos\frac{\Omega_R t}{2} - i\frac{\delta}{\Omega_R}\sin\frac{\Omega_R t}{2}\right)|1\rangle - ie^{-i\omega_2 t}e^{-i\omega t/2}\frac{\omega_R}{\Omega_R}\sin\frac{\Omega_R t}{2}|2\rangle\right]}$$

2. Density Matrix Formalism. We may parameterize the Hamiltonian

$$\mathcal{H} = -\vec{\mu}\cdot\vec{B} = \frac{\hbar}{2}\begin{pmatrix}\omega_0 & \omega_R e^{-i\omega t}\\ \omega_R e^{i\omega t} & -\omega_0\end{pmatrix}$$

in terms of the Pauli matrices as

$$\mathcal{H} = \frac{\hbar}{2}\left(\omega_R\cos(\omega t)\,\hat{\sigma}_x + \omega_R\sin(\omega t)\,\hat{\sigma}_y + \omega_0\,\hat{\sigma}_z\right).$$

In view of the von Neumann equation, we have

$$\begin{aligned}
i\hbar\dot{\rho} &= \frac{i\hbar}{2}(\dot{r}_x\,\hat{\sigma}_x + \dot{r}_y\,\hat{\sigma}_y + \dot{r}_z\,\hat{\sigma}_z)\\
&= [\mathcal{H},\rho]\\
&= \frac{\hbar}{4}[\omega_R\cos(\omega t)\,\hat{\sigma}_x + \omega_R\sin(\omega t)\,\hat{\sigma}_y + \omega_0\,\hat{\sigma}_z, r_x\,\hat{\sigma}_x + r_y\,\hat{\sigma}_y + r_z\,\hat{\sigma}_z].
\end{aligned}$$

where we have used the fact that $\rho = (\mathbb{I} + \vec{r}\cdot\vec{\sigma})/2$. By calculating each $\hat{\sigma}_i$ term in the commutator, we can find three differential equations for $\vec{r}$, each associated with a component r_i. Using the fact that

$$[\sigma_i,\sigma_j] = 2i\epsilon_{ijk}\sigma_k$$

we immediately find the following three equations:

$$\begin{aligned}
\hat{\sigma}_x: &\quad \dot{r}_x = \omega_R\sin(\omega t)r_z - \omega_0 r_y\\
\hat{\sigma}_y: &\quad \dot{r}_y = \omega_0 r_x - \omega_R\cos(\omega t)r_z\\
\hat{\sigma}_z: &\quad \dot{r}_z = \omega_R\cos(\omega t)r_y - \omega_R\sin(\omega t)r_x
\end{aligned}$$

If we now call

$$\vec{\Omega} = (\Omega_x,\Omega_y,\Omega_z) = (\omega_R\cos(\omega t), \omega_R\sin(\omega t), \omega_0)^\top$$

then it is clear that

$$\dot{r}_i = \epsilon_{ijk}\Omega_j r_k.$$

In other words,

$$\frac{d\vec{r}}{dt} = \vec{\Omega} \times \vec{r},$$

as desired. This is a nice result which states that the motion of the **Bloch vector** $\vec{r}$ for a generic two-level system whose Hamiltonian takes the form $\mathcal{H} = -\vec{\Omega} \cdot \vec{B}$ is given by $d\vec{r}/dt = \vec{\Omega} \times \vec{r}$ where $|\vec{r}|$ is a constant and $\vec{r}$ precesses about $\vec{\Omega}$. Through this particular example we also see that the motion of the Bloch vector for a two-level system subjected to some off-diagonal perturbation corresponds exactly to that of a classical magnetic moment in a magnetic field.

Notice further that we have made no assumption about the purity of the system. The fact that $|\vec{r}|$ remains constant in time implies that the purity $\mathrm{Tr}(\rho^2) = (1 + |\vec{r}|^2)/2$ is also constant, i.e. unitary (Hamiltonian) time evolution preserves the purity. In the special case where ρ describes a pure state, we see immediately that the system remains a pure state.

3. Atomic Units.

a) Given $E_A = e/a_0^2$, the energy of the electrostatic potential is given by

$$\mathcal{E}_{\text{stat}} = \frac{e}{a_0^2} \times (ea_0) = \frac{e^2}{a_0}.$$

The energy due to quantum confinement may be assumed to be the kinetic energy of the electron, which comes from an angular momentum of $\sim \hbar$, and so

$$\mathcal{E} \sim mv^2 = m\left(\frac{L}{ma_0}\right)^2 = \frac{\hbar^2}{ma_0^2}.$$

Equating these two energies we find

$$a_0 = \frac{\hbar^2}{m_e e^2}.$$

For comparison, the SI-unit definition for the Bohr radius is

$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2},$$

which we would have gotten if we were using SI units instead.

b) Suppose that we have an electron is orbiting a proton in a circle of radius a_0. We may treat this as a current and calculate the magnetic field produced at the center. Biot-Savart law says that

$$dB = \frac{\mu_0 I d\vec{l} \times \vec{r}}{4\pi r^2} = \frac{\mu_0 I}{4\pi a_0^2}\, dl$$

at the center. Here the current I may be computed via

$$I = \frac{e}{\tau} = \frac{ev}{2\pi a_0} = \frac{e}{2\pi a_0}\frac{\hbar}{ma_0} = \frac{e\hbar}{2\pi m a_0^2}$$

where we have assumed once again that the electron has angular momentum $L = \hbar = mva_0$. Plugging I into the preceding equation and integrate over the electron orbit we find that

$$B_N = \oint dB = 2\pi a_0 \frac{\mu_0}{4\pi a_0^2}\frac{e\hbar}{2\pi m_e a_0^2} = \frac{\mu_0 e\hbar}{4\pi m_e a_0^3}.$$

c) The interaction energy between a Bohr magneton and a magnetic field B_H is given by

$$E = \mu_B B_H = \frac{e\hbar}{2m_e c} B_H$$

The Hartree is given by

$$E_H = \frac{\hbar^2}{m_e a_0^2}.$$

Setting $E_H = E$ gives

$$B_H = \frac{\hbar^2}{m_e a_0^2} \frac{2m_e c}{e\hbar} = 2\left(\frac{\hbar c}{e^2}\right)\frac{e}{a_0^2}.$$

d) In Part (c) we have written our answer to suggest that

$$\boxed{B_H = \frac{2}{\alpha} E_A}$$

where $\alpha = e^2/\hbar c$ is the fine structure constant. It remains to work out what B_N is in terms of E_A. To do this, we will substitute in the expression for a_0:

$$B_N = \frac{\mu_0}{4\pi}\frac{\hbar}{m_e}\frac{m_e e^2}{4\pi\epsilon_0\hbar^2}\frac{e}{a_0^2} = \frac{\mu_0}{4\pi}\frac{e^2}{4\pi\epsilon_0\hbar}\frac{e}{a_0^2} = \left(\frac{\mu_0}{4\pi}\frac{e^2}{4\pi\epsilon_0\hbar}\right)E_A.$$

In atomic units, $\hbar = m_e = e = 4\pi\epsilon_0 = 1$, and so we have

$$B_N = \frac{\mu_0}{4\pi} E_A.$$

Finally, recall that

$$\frac{1}{\sqrt{\mu_0\epsilon_0}} = c \implies c = \frac{1}{\sqrt{\frac{\mu_0}{4\pi}4\pi\epsilon_0}} \implies \frac{\mu_0}{4\pi} = \frac{1}{4\pi\epsilon_0}\frac{1}{c^2}.$$

Now, the speed of light c can be written in terms of the fine structure constant:

$$c = \frac{e^2}{4\pi\epsilon_0\hbar\alpha} = \frac{1}{\alpha}$$

in atomic units. As a result, we have that

$$\frac{\mu_0}{4\pi} = \alpha^2.$$

From here, we find

$$\boxed{B_N = \alpha^2 E_A}$$

e) Since the