Problem Set 2

1 Rabi problem [8 pts]

Let $\omega_2 - \omega_1 = \omega_0$ be the resonance frequency and $H = H_0 + H'(t)$ be the total Hamiltonian for time-independent $H_0 = \frac{\omega_0}{2}(|2\rangle\langle 2| - |1\rangle\langle 1|)$ and time-dependent $H'(t) = \frac{\omega_R}{2}(e^{i\omega t} + e^{-i\omega t})|1\rangle\langle 2| + \text{h.c.}$ We set $\hbar = 1$.

a) There are several ways to solve the equations of motion:

1) Obtain a 2nd order differential equation for a_1 or a_2. It will have constant coefficients.

2) Change variables to $b_2 = a_2 e^{i(\omega - \omega_0)t/2}$, and $b_1 = a_1 e^{i(\omega_0 - \omega)t/2}$. The resulting equations of motion will be time-independent. You can solve them by finding eigenvectors and eigenvalues of the ODE matrix. You can think of this as a transformation to the frame rotating at the frequency of the drive ω. As seen in the class notes, this transformation will give you a new Hamiltonian

$$\tilde{H} = T^\dagger H T - i T^\dagger \dot{T} \tag{1}$$

where the unitarity transformation T is a simple rotation about the spinor z-axis, generated by the spin angular momentum operator S_z. Rotating along $\theta = -\omega t$ gives

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

for Pauli matrix σ_z. When we do this, we find that there are exponentials in the off-diagonal terms that vary as $e^{\pm 2i\omega t}$. In order for us to be able to drop the exponentials, the 2ω terms must evolve much faster than the dynamics we are interested in, which occur at Ω_R; otherwise, it too would couple into the system, and we can no longer ignore its effects on the evolution of our state. However, because we have taken $|\delta|$, $\omega_R \ll \omega_0$, we know that $\Omega_R = \sqrt{\delta^2 + \omega_R^2} \ll \omega_0$ which allows us to drop the fast-varying component of the cos drive.

3) Plug in $a_2(t) = A_2 e^{i\Omega_2 t}$ and $a_1(t) = A_1 e^{i\Omega_1 t}$. Find two solutions and take their linear combination. Imposing the initial conditions replaces the general pre-factors with expressions in terms of $a_1(0) = 1$ and $a_2(0) = 0$.

The result is:

$$
\begin{aligned}
a_2(t) &= \frac{\Omega_R - \delta}{2\Omega_R} e^{-\frac{1}{2}i(\delta+\Omega_R)t} - \frac{\omega_R}{2\Omega_R} e^{-\frac{1}{2}i(\delta-\Omega_R)t} \\
a_1(t) &= \frac{\Omega_R + \delta}{2\Omega_R} e^{\frac{1}{2}i(\delta-\Omega_R)t} + \frac{\Omega_R - \delta}{2\Omega_R} e^{\frac{1}{2}i(\delta+\Omega_R)t}
\end{aligned}
\tag{3}
$$

which gives the wave function

$$
\begin{aligned}
|\psi(t_1)\rangle &= a_1(t_1)|1\rangle + a_2(t_1)|2\rangle \\
&= e^{i\delta t_1/2}\left[\cos\left(\frac{\Omega_R t_1}{2}\right) - i\frac{\delta}{\Omega_R}\sin\left(\frac{\Omega_R t_1}{2}\right)\right]|1\rangle - ie^{-i\delta t_1/2}\frac{\omega_R}{\Omega_R}\sin\left(\frac{\Omega_R t_1}{2}\right)
\end{aligned}
\tag{4}
$$

where $\Omega_R = \sqrt{\delta^2 + \omega_R^2}$ and $\delta = \omega - \omega_0$.

b) Using our solution for the state in part (a) we find the probability to be in state $|2\rangle$ at time t_1 is

$$
P_2(t_1) = |\langle 2|\psi(t_1)\rangle|^2 = \frac{\omega_R^2}{\Omega_R^2}\sin^2\left(\frac{\Omega_R t_1}{2}\right)
\tag{5}
$$

c) The state evolves in the bare Hamiltonian $H_0 = \frac{\omega_0}{2}\sigma_z$. We evolve each of the eigenstates $|1\rangle$ and $|2\rangle$

$$
\begin{aligned}
|\psi(t_1 + T)\rangle &= \left[e^{i(\delta t_1 + \omega_0 T)/2}\cos\left(\frac{\Omega_R t_1}{2}\right) - i\frac{\delta}{\Omega_R}\sin\left(\frac{\Omega_R t_1}{2}\right)\right]|1\rangle \\
&\quad - ie^{-i(\delta t_1 + \omega_0 T)/2}\frac{\omega_R}{\Omega_R}\sin\left(\frac{\Omega_R t_1}{2}\right)|2\rangle
\end{aligned}
\tag{6}
$$

2   Density matrix formalism [6 pts]

From observation (again setting $\hbar = 1$)

$$
\begin{aligned}
V_1 &= \frac{\omega_R}{2}\cos(\omega t) \\
V_2 &= \frac{\omega_R}{2}\sin(\omega t).
\end{aligned}
\tag{7}
$$

Using the von Neumann EOM, we find

$$
\begin{aligned}
\dot{\vec{r}} &= \frac{1}{i}[H, \vec{r} \cdot \vec{\sigma}] \\
&= \frac{1}{2i}[\Omega_j \sigma_j, r_k \sigma_k] \\
&= \frac{1}{2i}\Omega_j r_k [\sigma_j, \sigma_k] \\
&= \frac{1}{2i}\Omega_j r_k (2i\varepsilon_{jkl}\sigma_l) \\
&= \varepsilon_{jkl}\Omega_j r_k \sigma_l \\
&= \vec{\Omega} \times \vec{r}.
\end{aligned}
\tag{8}
$$

This EOM simply describes classical precession of a vector $\vec{r}$ about the axis $\vec{\Omega}$!

3   Atomic units [6 pts]

Let the atomic unit of E field be $E_A \equiv e/a_0^2$, the field of the ground state of the electron at the site of the proton in hydrogen. In the following we use cgs units. To convert to SI, replace $e^2 \to e^2/4\pi\epsilon_0$. Factors of 2 are ignored.

a) An electron of mass m is confined to a width $\Delta x = a_0$. Using the lower bound for the uncertainty principle (and ignoring factors of 2) we find $\Delta p = \hbar/a_0$ (equivalently its wavevector is $k = 1/a_0$). This confinement imparts a kinetic energy T to the electron

$$
T \sim \frac{p^2}{m} \sim \frac{\hbar^2 k^2}{m} \sim \frac{\hbar^2}{ma_0^2}.
\tag{9}
$$

Equating this with one Hartree e^2/a_0 yields

$$
a_0 = \frac{\hbar^2}{me^2}
\tag{10}
$$

which is in fact the Bohr radius.

b) Classically, the nucleus sees the orbiting electron as a current loop with radius a_0, carrying current $I = e/T$ where $T = 2\pi a_0/v$ is the period of the electron's orbit. At its center, this loop produces magnetic field

$$
B_N = \frac{2\pi I}{ca_0} = \frac{e}{a_0^2}\frac{v}{c} = \alpha E_A
\tag{11}
$$

c) A Bohr magneton is

$$\mu_B = \frac{e\hbar}{2mc} \sim \alpha e a_0. \tag{12}$$

Equate $\mu_B B_H$ with one Hartree to get

$$B_H \sim \frac{1}{\alpha}\frac{e}{a_0^2} = \frac{E_A}{\alpha} \tag{13}$$

d) See parts (b) and (c).

e) B_N corresponds to the magnetic field produced by the orbiting electron in a hydrogen atom and as such gives the typical scale of magnetic fields due to motion of atomic charges. This makes it the preferred choice for an atomic unit of magnetic field.

Since the hydrogen electron moves at velocity α smaller than the speed of light, the magnetic field B_N that it produces is a factor of α times smaller than its electric field E_A. In SI units:

$$B_N = \frac{e}{4\pi\epsilon_0}\frac{\alpha}{a_0}\frac{1}{c} = 12.52\,\text{T} \tag{14}$$

At this practically accessible field, the Zeeman interaction with the external field becomes comparable to even the strongest magnetic coupling in atoms ($L \cdot S$ coupling).

A Bohr magneton corresponds to the magnetic moment of the hydrogen electron's orbital motion. Therefore, B_H corresponds to the magnetic field which interacts with this electron on the same energy scale as the nuclear electric field. Since the hydrogen electron moves α times slower than the speed of light, $B_H \gtrsim 10^5\,\text{T}$ is $1/\alpha$ times larger than E_A and $1/\alpha^2$ times larger than B_N, i.e. more than 4 orders of magnitude larger than both the atomic and the highest laboratory magnetic fields.