Physics 531 Homework 8

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2. *Rabi oscillations.* Consider a spin-1/2 particle in a magnetic field $\vec{B} = B_0\hat{z}$ such that the spin eigenstates are split in energy by $\hbar\omega_0$ (let's label the ground state $|0\rangle$ and the excited state $|1\rangle$). The Hamiltonian for the system is written as

$$H_{\text{Zeeman}} = -\frac{\hbar\omega_0}{2}\sigma_z;$$

here and below, $\sigma_{x,y,z}$ are the usual Pauli matrices. A second, oscillating field is applied in the transverse plane, giving rise to a time-dependent term in the Hamiltonian

$$H_{\text{Rabi}} = \frac{\hbar\omega_1}{2}(\cos\omega t\,\sigma_x - \sin\omega t\,\sigma_y),$$

where ω_1 parameterizes the strength of the oscillating transverse field and where in general $\omega_1 \neq \omega_0$.

(a) Construct the 2×2 Hamiltonian matrix.

(b) Use the time-dependent unitary transformation $U = e^{(i\omega t/2)\sigma_z}$ to transform to a reference frame rotating with the oscillating transverse field. Recall that a state $|\psi\rangle$ in the laboratory frame is transformed to the state $\tilde{\psi} = U\psi$ in the rotating frame. Evaluate the time derivative $d\tilde{\psi}/dt$ to derive the Schrodinger equation in the rotating frame. What is the effective Hamiltonian in the rotating frame?

(c) Take the initial state $|\psi(t=0)\rangle = |0\rangle$. Compute the time evolution of the state in the rotating frame for arbitrary detuning $\Delta = \omega - \omega_0$ of the drive frequency from the Larmor frequency. Feel free to do this numerically. If you take a numerical approach, generate a surface plot of $\langle\sigma_z\rangle$ versus time and drive detuning. If you take an analytic approach, derive an expression for $|\tilde{\psi}(t)\rangle$ as a function of Δ and use this to compute $\langle\sigma_z\rangle(t;\Delta)$. Again, work in the rotating frame, where H_{eff} is time-independent. (Otherwise this problem will be very difficult!)

Solution:

(a)

$$\begin{aligned} H &= \frac{-\hbar\omega_0}{2}\sigma_z + \frac{\hbar\omega_1}{2}(\cos\omega t\,\sigma_x - \sin\omega t\,\sigma_y) \\ &= \frac{\hbar}{2}\begin{pmatrix} -\omega_0 & \omega_1(\cos\omega t - i\sin\omega t) \\ \omega_1(\cos\omega t - i\sin\omega t) & \omega_0 \end{pmatrix} \end{aligned}$$

$$\boxed{H = \frac{\hbar}{2}\begin{pmatrix} -\omega_0 & \omega_1 e^{i\omega t} \\ \omega_1 e^{i\omega t} & \omega_0 \end{pmatrix}}$$

(b) In order to find the effective Hamiltonian, we must transform the time-dependent Schrodinger equation into the rotating frame using the unitary transformation $U = e^{(i\omega t/2)\sigma_z}$. Notice that

$$
\begin{aligned}
i\hbar\frac{d\psi}{dt} &= \hat{H}\psi, \\
\dot{U} &= \frac{-i\omega}{2}\sigma_z U, \\
\dot{\psi} &= \frac{1}{i\hbar}\hat{H}\psi
\end{aligned}
$$

Transforming ψ into $\tilde{\psi} = U\psi$, we can evaluate the right hand side of the Schrodinger equation using the chain rule.

$$
\begin{aligned}
i\hbar\frac{d}{dt}(U\psi) &= i\hbar[\dot{U}\psi + U\dot{\psi}] \\
&= i\hbar[\frac{-i\omega}{2}\sigma_z U\psi + \frac{1}{i\hbar}\hat{H}\psi \\
&= \frac{\hbar\omega}{2}\sigma_z U\psi + U\hat{H}U^\dagger U\psi \\
&= \frac{\hbar\omega}{2}\sigma_z\tilde{\psi} + \tilde{H}\tilde{\psi}
\end{aligned}
$$

This is the Schrodinger equation for our rotating frame with

$$
\begin{aligned}
\tilde{H} &= U\hat{H}U^\dagger \\
&= \frac{\hbar}{2}e^{\frac{-i\omega t}{2}\sigma_z}\begin{pmatrix} -\omega_0 e^{\frac{i\omega t}{2}} & \omega_1 e^{\frac{i\omega t}{2}} \\ -\omega_1 e^{\frac{-i\omega t}{2}} & -\omega_0 e^{\frac{i\omega t}{2}} \end{pmatrix} \\
&= \frac{\hbar}{2}\begin{pmatrix} -\omega_0 & \omega_1 \\ \omega_1 & \omega_0 \end{pmatrix}
\end{aligned}
$$

and we can read off the effective Hamiltonian.

$$
H_{\text{eff}} = \frac{\hbar\omega}{2} + \tilde{H}
$$

$$
\boxed{H_{\text{eff}} = \frac{\hbar}{2}\begin{pmatrix} \omega - \omega_0 & \omega_1 \\ \omega_1 & -(\omega - \omega_0) \end{pmatrix}}
$$

(c) Let the Rabi frequency ω_R be the field oscillation frequency ω_1 plus some arbitrary detuning Δ. The values add in quadrature since they are all vectors.

$$
\omega_R = \sqrt{\Delta^2 + \omega_1^2}
$$

In terms of this frequency, the Rabi time evolution operator becomes

$$
\begin{aligned}
U_{\text{Rabi}} &= \exp\frac{-i\omega_R t}{2}\left(\frac{\Delta}{\omega_R}\sigma_z + \frac{\omega_1}{\omega_R}\sigma_x\right) \\
&= \begin{pmatrix} c - is\frac{\Delta}{\omega_R} & -is\frac{\omega_1}{\omega_R} \\ -is\frac{\omega_1}{\omega_R} & c + is\frac{\Delta}{\omega_R} \end{pmatrix}
\end{aligned}
$$

where $c \equiv \cos\frac{\omega_R t}{2}$ and $s \equiv \sin\frac{\omega_R t}{2}$. To find the time evolution of our initial state, we just apply this operator.

$$|\psi(t=0)\rangle = |0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$
$$|\psi(t)\rangle = U_{\text{Rabi}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} c - is\frac{\Delta}{\omega_R} \\ -is\frac{\omega_1}{\omega_R} \end{pmatrix}$$

Using this time evolved state, we can solve for $\langle \sigma_z \rangle$ in the typical fashion.

$$\begin{aligned}
\langle \sigma_z \rangle &= \langle \psi | \sigma_z | \psi \rangle \\
&= \begin{pmatrix} c - is\frac{\Delta}{\omega_R} & -is\frac{\omega_1}{\omega_R} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} c - is\frac{\Delta}{\omega_R} \\ -is\frac{\omega_1}{\omega_R} \end{pmatrix} \\
&= c^2 + s^2\frac{\Delta^2}{\omega_R^2} - s^2\frac{\omega_1^2}{\omega_R^2}
\end{aligned}$$
$$\boxed{\langle \sigma_z \rangle = \cos^2\left(\frac{\sqrt{\Delta^2+\omega_1^2}\,t}{2}\right) + \sin^2\left(\frac{\sqrt{\Delta^2+\omega_1^2}\,t}{2}\right)\left[\frac{\Delta^2-\omega_1^2}{\Delta^2+\omega_1^2}\right]}$$

3. *Inhomogeneous broadening.* Consider an ensemble of spins initialized in the state $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$. Each spin is subjected to a slightly different Zeeman field, so that the distribution of detunings Δ from the average Larmor frequency ω_0 is given by

$$P(\Delta) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\Delta^2/2\sigma^2}$$

here σ is the standard deviation of the distribution of Larmor frequencies (not a Pauli matrix! - beware the clash of notation), due for example to an inhomogeneous magnetic field across the spin sample. Work in a reference frame rotating at the average Larmor frequency ω_0.

(a) In this reference frame, what is the Hamiltonian for a single spin whose Larmor frequency is detuned by Δ from ω_0? What is the unitary time evolution operator?

(b) Calculate the time-evolved state for a single spin with detuning Δ in this rotating frame. *Hint.* For $\Delta = 0$, the state will not evolve in time. Calculate $\langle \sigma_x \rangle (t; \Delta)$ for a single spin at detuning Δ.

(c) Now average your answer for $\langle \sigma_x \rangle (t; \Delta)$ over the whole spin ensemble to compute what is called in the NMR world the "free induction decay" of the sample. The decay of the signal is due to rapid loss of phase coherence as different spins precess at different rates. In the Fourier domain, this corresponds to a broad spectral response. Broadening of the resonant response due to extrinsic effects (such as a nonuniform magnetic field) is known as inhomogeneous broadening. In this example, the phase coherence time of the individual spins in the ensemble is infinite (we have not yet talked about how to treat decoherence of quantum systems). In the case of inhomogeneous broadening, it turns out that it is possible to play some tricks to "resurrect" the coherent magnetization of the spin ensemble long after the free induction signal has decayed away to zero.

(d) Now consider the following spin echo sequence (still in the rotating frame): free evolution for fixed time $\tau - \pi$ rotation about $x -$ free evolution for variable time t Construct the unitary operator that describes this evolution. For a single spin with detuning $Delta$, construct the time-evolved state.

(e) For the spin echo sequence, average $\langle \sigma_x \rangle (t; \Delta)$ over the whole spin ensemble to compute the echo signal. Sketch or plot the echo signal for the range $(t - 5/\sigma, t + 5/\sigma)$. Explain.

Solution:

(a) H_{eff} and U_{Rabi} are the same as in the previous question.

$$H_{\text{eff}} = \frac{\hbar}{2}\begin{pmatrix} \omega-\omega_0 & \omega_1 \\ \omega_1 & -(\omega-\omega_0) \end{pmatrix}$$

$$U_{\text{Rabi}} = \begin{pmatrix} c - is\frac{\Delta}{\omega_R} & -is\frac{\omega_1}{\omega_R} \\ -is\frac{\omega_1}{\omega_R} & c + is\frac{\Delta}{\omega_R} \end{pmatrix}$$

(b) The initial state

$$|\psi(t=0)\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

transforms into

$$|\psi(t)\rangle = U\psi = \frac{1}{\sqrt{2}}\begin{pmatrix} c - is\frac{\Delta+\omega_1}{\omega_R} \\ c + is\frac{\Delta-\omega_1}{\omega_R} \end{pmatrix}$$

From this, we can compute $\langle\sigma_x\rangle$

$$\begin{aligned}
\langle\sigma_x\rangle &= \langle\psi|\sigma_x|\psi\rangle \\
&= \frac{1}{2}\begin{pmatrix} c - is\frac{\Delta+\omega_1}{\omega_R} & c + is\frac{\Delta-\omega_1}{\omega_R} \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} c - is\frac{\Delta+\omega_1}{\omega_R} \\ c + is\frac{\Delta-\omega_1}{\omega_R} \end{pmatrix} \\
&= \frac{1}{2}\Bigg[c^2 + ics\left(\frac{\Delta+\omega_1}{\omega_R}\right) + ics\left(\frac{\Delta-\omega_1}{\omega_R}\right) - s^2\left(\frac{\Delta+\omega_1}{\omega_R}\right)\left(\frac{\Delta-\omega_1}{\omega_R}\right) \\
&\qquad + c^2 - ics\left(\frac{\Delta+\omega_1}{\omega_R}\right) - ics\left(\frac{\Delta-\omega_1}{\omega_R}\right) - s^2\left(\frac{\Delta+\omega_1}{\omega_R}\right)\left(\frac{\Delta-\omega_1}{\omega_R}\right)\Bigg] \\
&\boxed{\langle\sigma_x\rangle = c^2 - s^2\frac{\Delta-\omega_1}{\Delta+\omega_1}}
\end{aligned}$$

where again $c \equiv \cos\frac{\omega_R t}{2}$ and $s \equiv \sin\frac{\omega_R t}{2}$. As a check, we can plug in $\Delta = 0$ and notice that $\langle\sigma_x\rangle = c^2 + s^2 = 1$, which is expected for a system with no detuning.

(c) Averaging over the entire spin ensemble, we get

$$\begin{aligned}
\langle\sigma_x\rangle_{\text{avg}} &= \int_{-\infty}^{\infty} \langle\sigma_x\rangle\, P(\Delta) d\Delta \\
&= \int_{-\infty}^{\infty} \left(\cos^2\frac{\omega_R t}{2} - \sin^2\frac{\omega_R t}{2}\left(\frac{\Delta-\omega_1}{\Delta+\omega_1}\right)\right)\frac{1}{\sqrt{2\pi\sigma^2}}e^{-\Delta^2/2\sigma^2} d\Delta
\end{aligned}$$

which evaluates to

$$\boxed{\langle\sigma_x\rangle_{\text{avg}} = e^{-\sigma^2 t^2/2}}$$

(d) Our unitary operator is U_{Rabi} for all times other than when $t = \tau$. At this time, we to a unitary rotation about x, described by $U = \exp\frac{-i\pi}{\hbar}\hat{x}\vec{S}$ where $\vec{S}$ is the spin matrix. This can be written as the following conditional statement.

$$U = \begin{cases} U_{\text{Rabi}}, & \text{for } t \neq \tau \\ \exp\frac{-i\pi}{\hbar}\hat{x}\vec{S}, & \text{for } t = \tau \end{cases}$$

$$= \begin{cases} U_{\text{Rabi}}, & \text{for } t \neq \tau \\ \exp\frac{-i\pi}{\hbar}\sigma_x, & \text{for } t = \tau \end{cases}$$

After evolution, our initial state then becomes

$$|\psi(t=0)\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$$

$$\boxed{|\psi(t)\rangle = \begin{cases} \frac{1}{\sqrt{2}}\begin{pmatrix} c - is\frac{\Delta+\omega_1}{\omega_R} \\ c + is\frac{\Delta-\omega_1}{\omega_R}\end{pmatrix}, & \text{for } t \neq \tau \\ \frac{1}{\sqrt{2}}\exp\frac{-i\pi}{\hbar}\sigma_x \begin{pmatrix} c - is\frac{\Delta+\omega_1}{\omega_R} \\ c + is\frac{\Delta-\omega_1}{\omega_R}\end{pmatrix}, & \text{for } t = \tau \end{cases}}$$

This makes sense, as our state is identical to the state in part b until the time τ, after which it it simply multiplied by the unitary rotation operator.

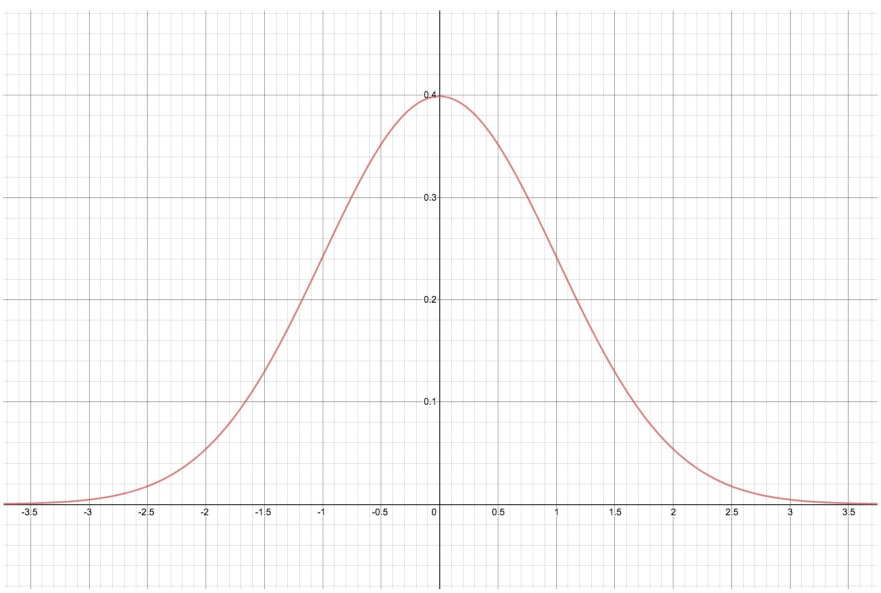
(e)

$$\boxed{\langle\sigma_x\rangle = c^2 - s^2\frac{\Delta-\omega_1}{\Delta+\omega_1} \text{ for all t}}$$

since the rotation drops out of the expectation value:

$$e^{\frac{-i\pi}{\hbar}\sigma_x}\langle\psi|\sigma_x e^{\frac{-i\pi}{\hbar}\sigma_x}|\psi\rangle = e^0\langle\psi|\sigma_x|\psi\rangle = \langle\psi|\sigma_x|\psi\rangle$$

$$\begin{aligned}\langle\sigma_x\rangle_{\text{avg}} &= \int_{-\infty}^{\infty}\langle\sigma_x\rangle P(\Delta)d\Delta \\ &= \int_{-\infty}^{\infty}\left(\cos^2\frac{\omega_R t}{2} - \sin^2\frac{\omega_R t}{2}\left(\frac{\Delta-\omega_1}{\Delta+\omega_1}\right)\right)\frac{1}{\sqrt{2\pi\sigma^2}}e^{-\Delta^2/2\sigma^2}d\Delta\end{aligned}$$



The distribution of Δ is gaussian, so the echo signal will also be gaussian.