Problem Set 2

Due: Friday 5pm, Feb 18, via Canvas upload or in envelope outside 26-255
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Office hours TBA, in 26-214 (CUA seminar room)

1 Rabi problem [8 pts]

A two-state system is in the state $|1\rangle$ at $t = 0$. An oscillating field is applied at frequency ω with coupling matrix element $\langle 2|H'(t)|1\rangle = \hbar\omega_R \cos\omega t$. The eigenenergies of the states $|1\rangle$ and $|2\rangle$ are $\hbar\omega_1$ and $\hbar\omega_2$, respectively. Assume that $\omega_R \ll \omega_2 - \omega_1$, and $\omega_2 > \omega_1$.

a) Using the rotating wave approximation (see below), find the wave function for the system at $t_1 > 0$.

b) What is the probability that the system will be found in state $|2\rangle$ if a measurement is made at t_1?

c) The oscillating field is turned off at t_1. What is the time-dependent wave function at later times?

Hint: One can decompose the off-diagonal terms of the Hamiltonian into terms involving $e^{\pm i\omega t}$. There are terms that are "in sync" with the free evolution of the system in the absence of the drive, i.e. they approximately co-rotate with the pseudo-spin we use to represent this 2-level problem, causing near-resonant transitions. There are also terms that are counter-rotating with the pseudo-spin, they are far off-resonant and cause only small-amplitude, rapidly oscillating behavior, which you can neglect. This is the rotating wave approximation.

2 Density Matrix formalism [6 pts]

Preamble: The Hamiltonian of a magnetic moment $\vec{\mu}$ in a combination of a static and a rotating field, $\vec{B}(t) = -(B_1\cos\omega t, B_1\sin\omega t, B_0)$ is

$$H = -\vec{\mu}\cdot\vec{B} = \frac{\hbar}{2}\begin{pmatrix} \omega_0 & \omega_R\, e^{-i\omega t} \\ \omega_R\, e^{i\omega t} & -\omega_0 \end{pmatrix}. \tag{1}$$

Here $\omega_0 = \gamma B_0$ and $\omega_R = \gamma B_1$ are the Larmor and the Rabi frequency associated with the static field B_0 and the rotating field of magnitude B_1, respectively, and γ is the gyromagnetic ratio. The basis is $\begin{pmatrix} 1 \\ 0 \end{pmatrix} = |\downarrow\rangle \equiv |e\rangle$, $\begin{pmatrix} 0 \\ 1 \end{pmatrix} = |\uparrow\rangle \equiv |g\rangle$, where $|\uparrow\rangle, |\downarrow\rangle$

are the states where $\vec{\mu}$ is oriented along the $\mp z$ axis. The time evolution of any state $|\psi(t)\rangle = a_g(t)\,|g\rangle + a_e(t)\,|e\rangle$ is determined by the two coefficients $a_g(t), a_e(t)$, and we solved this problem in class.

The Schrödinger equation describes unitary time evolution, so it leaves the system in a "pure" state. It cannot describe decoherence, or uncontrolled loss of atoms, phase, etc. This is why we need the density matrix formalism. For a pure state, the density matrix is $\rho = |\psi\rangle\langle\psi|$, for an ensemble it is $\rho = \sum_i p_i\,|\psi_i\rangle\langle\psi_i|$. For this two-level system, a general density matrix will be represented by a generic 2×2 matrix, which we can conveniently construct out of the unity operator $\mathbb{1}$ and the three Pauli spin matrices

$$\widehat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \widehat{\sigma}_x = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \widehat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{2}$$

One can thus write $\rho = \frac{1}{2}\left(r_0\mathbb{1} + r_x\widehat{\sigma}_x + r_y\widehat{\sigma}_y + r_z\widehat{\sigma}_z\right) = \frac{1}{2}\left(r_0\mathbb{1} + \vec{r}\cdot\vec{\sigma}\right)$, and since $\mathrm{Tr}\rho = r_0 = \sum_i p_i = 1$ we have

$$\rho = \frac{1}{2}\left(\mathbb{1} + \vec{r}\cdot\vec{\sigma}\right) \tag{3}$$

with *real* vector $\vec{r}$, called the Bloch vector, which lies inside the unit sphere. For pure states one has $r_x^2 + r_y^2 + r_z^2 = 1$, so they are described by Bloch vectors that lie on the surface of the unit sphere. Mixed states have smaller magnitude of $\vec{r}$.

Your task: Parameterize the Hamiltonian H above as

$$H = \frac{\hbar}{2}[V_1\widehat{\sigma}_x + V_2\widehat{\sigma}_y + \omega_0\widehat{\sigma}_z] \tag{4}$$

(Note that V_1, V_2 are going to be time-dependent).

Employing the von Neumann equation

$$i\hbar\dot{\rho} = [H, \rho] \tag{5}$$

show that $\vec{r}$ obeys the relation $\frac{d\vec{r}}{dt} = \vec{\Omega}\times\vec{r}$ with $\vec{\Omega} = V_1\hat{x} + V_2\hat{y} + \omega_0\hat{z}$. Can you interpret this result?

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 electron at the site of the proton in hydrogen.

a) On the scale of atomic units, the energy of the electrostatic potential balances the energy of quantum confinement. Use this equality to derive the atomic size, a_0. (Ignore numerical factors.)

b) Find the magnetic field of the electron at the proton, B_N. (Assume a classical orbit for the electron. If factors of 2 arise, ignore them.)

c) Find the magnetic field, B_H, which has an interaction energy of one Hartree with a Bohr magneton.

d) Express these fields in terms of E_A (Gaussian units).

e) Are there strong reasons to prefer B_N or B_H as the atomic unit of magnetic field?