Problem set 4

4.1 Density operators

A density operator of a two-level system can be represented by a 2×2 density matrix in the form

$$\hat{\rho} = \frac{1}{2}(\mathbb{1} + \mathbf{r} \cdot \boldsymbol{\sigma}) \,, \quad |\mathbf{r}| \leq 1 \tag{1}$$

where $\mathbb{1}$ is the 2×2 identity matrix, $\mathbf{r}$ is a vector in three dimensions and $\boldsymbol{\sigma}$ is a vector operator with the Pauli matrices as the Cartesian components.

a) Show that $\mathbf{r} = \langle \boldsymbol{\sigma} \rangle$.

b) If

$$\hat{\rho}_1 = \frac{1}{2}(\mathbb{1} + \mathbf{r}_1 \cdot \boldsymbol{\sigma}) \qquad \text{and} \qquad \hat{\rho}_2 = \frac{1}{2}(\mathbb{1} + \mathbf{r}_2 \cdot \boldsymbol{\sigma})$$

are two density matrices, show that the statistical mixture

$$\hat{\rho} = p_1 \hat{\rho}_1 + p_2 \hat{\rho}_2 = \frac{1}{2}(\mathbb{1} + \mathbf{r} \cdot \boldsymbol{\sigma})$$

with $\mathbf{r} = p_1 \mathbf{r}_1 + p_2 \mathbf{r}_2$.

c) Explain why this means that geometrically the set of all density matrices form of a sphere in three dimensions, with the pure states $|\mathbf{r}| = 1$ as the surface of the sphere (the Bloch sphere), and the mixed states as the interior of the sphere.

d) The density operator can also be expressed in bra-ket formulation as

$$\hat{\rho} = \rho_{11} \,|+\rangle\langle+| \;+\; \rho_{12} \,|+\rangle\langle-| \;+\; \rho_{21} \,|-\rangle\langle+| \;+\; \rho_{22} \,|-\rangle\langle-| \tag{2}$$

with $|\pm\rangle$ defined by $\sigma_z |\pm\rangle = \pm|\pm\rangle$.

What are the coefficients $\rho_{ij}, \; i, j = 1, 2$, expressed in terms of the Cartesian components x, y, z of $\mathbf{r}$?

e) Assume a spin-half system is prepared in a mixed state, with equal probability for *spin up* in the (positive) directions of the three coordinate axes x, y and z . Find the corresponding density matrix, expressed in the form (1). What is the von Neumann entropy of the state?

f) The above mixed state was realized as an ensemble of three different pure states (spin up along each of the three coordinate axes). Find at least one different ensemble of two or more pure states which gives the same density matrix.

4.2 Entropy of a thermal state

A thermal state is described by a temperature dependent density operator of the form

$$\hat{\rho} = N(\beta) \, e^{-\beta \hat{H}} \tag{3}$$

where $\beta = 1/(k_B T)$ with T as the temperature, k_B as the Boltzmann constant, and $N(\beta)$ as a normalization factor. This factor is given by

$$N(\beta)^{-1} = \mathrm{Tr}(e^{-\beta \hat{H}}) = \sum_k e^{-\beta E_k} \tag{4}$$

with E_k as the energy eigenvalues.

a) Show that the temperature dependent von Neumann entropy of this state can be expressed in terms of the normalization factor as

$$S(\beta) = \beta \frac{d}{d\beta} \log N(\beta) - \log N(\beta) \tag{5}$$

b) For a one-dimensional harmonic oscillator, with Hamiltonian

$$\hat{H} = \hbar\omega \sum_{n=0}^{\infty} (n + \frac{1}{2}) |n\rangle\langle n| \tag{6}$$

what is the expression for the temperature dependent entropy $S(\beta)$?

c) Plot S as a function of temperature, with $x = 2k_B T/(\hbar\omega)$ as the dimensionless temperature coordinate on the horizontal axis, for example in the interval $(0, 5)$. What are the asymptotic expressions for S in the limits $T \to 0$ ($\beta \to \infty$) and $T \to \infty$ ($\beta \to 0$). Comment on these results with reference to what we know about the values of the entropy for pure states and maximally mixed states. (Assume *log* in the definition of S to mean the natural logarithm.)

4.3 Bloch-Siegert shift

We consider first an electron in a constant external magnetic field in the z-direction subject to a rotating field in the xy-plane. The Hamiltonian has the form

$$H = \frac{\hbar}{2}\omega_0 \sigma_z + \frac{\hbar}{2} A(\cos(\omega t)\, \sigma_x + \sin(\omega t)\, \sigma_y)$$

Here ω_0 is the natural precession frequency of the electron spin in the external field, A is the amplitude of the driving field, and ω its frequency.

a) Show that by changing to a reference frame rotating with the frequency ω of the driving field, the total field is constant in the rotating frame. From the Hamiltonian in the rotating frame, conclude that resonance (in the sense of largest amplitude Rabi oscillations of the spin state if the initial state is the ground state) will take place when $\omega = \omega_0$ irrespective of the driving amplitude A.

Now we replace the rotating field by one oscillating in the x-direction, which in many cases is more realistic. The Hamiltonian now reads

$$H = \frac{\hbar}{2}\omega_0 \sigma_z + \frac{\hbar}{2} A \cos(\omega t) \sigma_x. \tag{7}$$

b) Show that using the same transformation as above, the Hamiltonian in the rotating frame will get an additional term which describes a field rotating at the frequency 2ω and give an explanation for why this happens. Explain why we in some cases to a good approximation can neglect this additional rotating component, and use the same Hamiltonian as we had for the rotating field also when the field is oscillating, which is usually called the rotating wave approximation.

We will now study how we can get more accurate results than what is obtained in the rotating wave approximation. To achieve this, we will start from the Hamiltonian (7), but instead of going to a rotating frame, we will make the transformation

$$|\psi'\rangle = e^{iS(t)}|\psi\rangle, \qquad S(t) = \frac{A}{2\omega}\xi\sin(\omega t)\,\sigma_x$$

where ξ is a parameter whose value we will choose later.

c) Show that the transformed Hamiltonian is

$$H' = \frac{\hbar}{2}\omega_0\left\{\cos\left[\frac{A}{\omega}\xi\sin(\omega t)\right]\sigma_z + \sin\left[\frac{A}{\omega}\xi\sin(\omega t)\right]\sigma_y\right\} + \frac{\hbar}{2}A(1-\xi)\cos(\omega t)\,\sigma_x.$$

Using the identities

$$\cos\left[\frac{A}{\omega}\xi\sin(\omega t)\right] = J_0\left(\frac{A}{\omega}\xi\right) + 2\sum_{k=1}^{\infty} J_{2k}\left(\frac{A}{\omega}\xi\right)\cos(2k\omega t)$$
$$\sin\left[\frac{A}{\omega}\xi\sin(\omega t)\right] = 2\sum_{k=0}^{\infty} J_{2k+1}\left(\frac{A}{\omega}\xi\right)\sin[(2k+1)\omega t]$$

where $J_k(x)$ is the Bessel function of the first kind of order k, one can find that $H' = H_0' + H_1' + H_2'$ with

$$H_0' = \frac{\hbar}{2}\omega_0 J_0\left(\frac{A}{\omega}\xi\right)\sigma_z$$
$$H_1' = \hbar\omega_0\sin(\omega t)J_1\left(\frac{A}{\omega}\xi\right)\sigma_y + \frac{\hbar}{2}A(1-\xi)\cos(\omega t)\sigma_x$$
$$H_2' = \hbar\omega_0\sum_{k=1}^{\infty}\left\{J_{2k}\left(\frac{A}{\omega}\xi\right)\cos(2k\omega t)\sigma_z + J_{2k+1}\left(\frac{A}{\omega}\xi\right)\sin[(2k+1)\omega t]\sigma_y\right\}.$$

You do not have to derive this. All the terms in H_2' have higher frequencies than the typical dynamical frequencies of the state, and we will ignore H_2' and approximate $H' \approx H_0' + H_1'$. We will also choose ξ so that it satisfies the equation

$$J_1\left(\frac{A}{\omega}\xi\right)\omega_0 = \frac{1}{2}A(1-\xi).$$

d) Explain what is special about this choice of ξ and why this simplifies the problem. Show that the resonance condition for large amplitude Rabi oscillations now is

$$\omega = \omega_0 J_0\left(\frac{A}{\omega}\xi\right). \tag{8}$$

e) According to Eq. (8), the resonance frequency now depends on the amplitude, in contrast to the case of a rotating field studied in question a). Use the series expansions for the Bessel functions

$$J_0(x) = 1 - \frac{x^2}{4} + \frac{x^4}{64} + \cdots$$
$$J_1(x) = \frac{x}{2} - \frac{x^3}{16} + \frac{x^5}{384} + \cdots$$

to show that in the limit of a weak driving field, $A \to 0$, we recover the resonance at $\omega = \omega_0$ as we had using the rotating wave approximation, and find the lowest order in A correction to the resonance frequency for small A.