

Week 3: Resonance and Decoherence Processes

1 Resonance in a QM System: Density Matrix Formalism

1.1 Density matrices - review

- We cannot describe processes like decoherence or loss of particles with Shroedinger equation as it deals only with pure states. The exception is when you have two states and all what happens is a loss to some other levels. Then Hamiltonian description can be used but eigenvalues have to be replaced by complex numbers. For processes like spontaneous emission density matrix approach have to be used.
- If we have a time dependent wave function:

$$|\Psi(t)\rangle = \sum_n c_n(t) |\Psi_n\rangle$$

then we can define arbitrary operators by matrices: $A_{nm} = \langle \Psi_n | \hat{A} | \Psi_m \rangle$. Expectation value of the operator is:

$$\langle \hat{A} \rangle_t = \langle \Psi(t) | \hat{A} | \Psi(t) \rangle = \sum_{m,n} c_m^*(t) c_n(t) A_{nm} = \sum_{m,n} \rho_{nm}(t) A_{nm} = Tr(\hat{\rho}(t) \hat{A})$$

with $\hat{\rho}(t) = |\Psi(t)\rangle \langle \Psi(t)|$ and the matrix element given by: $\rho_{nm} = c_m^*(t) c_n(t)$. The diagonal matrix elements ρ_{nn} are called the populations and the off-diagonal matrix elements ρ_{mn} are called coherences.

When we include the probabilities of being in a certain state to the density matrix description we get:

$$\hat{\rho}(t) = \sum_i P_i |\Psi(t)\rangle \langle \Psi(t)|$$

$$\langle \hat{A} \rangle_t = Tr(\hat{\rho}(t) \hat{A})$$

and we have two averages here; one is quantum mechanical expectation value and the other one is ensemble average with probability P_i .

- Using the Shroedinger equation we can derive an equation for density matrix:

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

- Properties of the density matrix:

$$Tr(\hat{\rho}) = \sum_i P_i = 1$$

$$Tr(\hat{\rho}^2) = \sum_i P_i^2 \leq 1,$$

for pure states:

$$Tr(\hat{\rho}^2) = \sum_i P_i^2 = 1.$$

Density matrix operator is hermitian.

- We want to use the density matrix for non-unitary time evolution. This is often the situation for smaller system that is open for a bigger system, where we limit our description to a small part of a larger system.

1.2 Density matrices formalism for arbitrary two-level systems

- The most general Hamiltonian for the most general two-level system can be constructed from Pauli matrices and the identity matrix. By appropriately shifting the zero-point energy we can use only Pauli matrices and we get:

$$\hat{H} = \frac{\hbar}{2}(\omega_1 \hat{\sigma}_x + \omega_2 \hat{\sigma}_y + \omega_3 \hat{\sigma}_z) = \frac{\hbar}{2} \boldsymbol{\omega} \cdot \hat{\boldsymbol{\sigma}}$$

- We describe two-level systems by density matrix which is also 2x2 matrix. The most general density matrix can also be expanded into those basic matrices. This time we can't throw away identity matrix because then there would be no trace and therefore no probability to find the particle.

$$\hat{\rho} = \frac{1}{2}(r_0 \hat{\mathbb{I}} + r_1 \hat{\sigma}_x + r_2 \hat{\sigma}_y + r_3 \hat{\sigma}_z) = \frac{1}{2}(\hat{\mathbb{I}} + \mathbf{r} \cdot \hat{\boldsymbol{\sigma}}),$$

because $Tr(\hat{\rho}) = r_0 = 1$. Vector \mathbf{r} is called the Bloch vector.

- We can insert those above formulas into the equation of motion to get:

$$\dot{\mathbf{r}} = \boldsymbol{\omega} \times \mathbf{r}$$

This equation tells us that an arbitrary two-level system with an arbitrary Hamiltonian can be regarded as a system where we have a vector \mathbf{r} which undergoes precession.

- Pure state will stay pure forever, because: $Tr(\hat{\rho}^2) = \frac{1}{2}[r_0^2 + |\mathbf{r}|^2] = const$. This is because $r_0 = 1$ and from the equation of motion we get that the length of the vector is not changing. This does not describe loss of coherence (decoherence).

2 Relaxation and the Bloch Equations

2.1 Relaxation - the Bloch equations

- Everything has to come to thermal equilibrium if we will wait for ever. So after long time the density matrix will thermalize to: $\hat{\rho}^T = \frac{1}{Z} e^{-H_0/kT}$ where Z is a partition function. No matter with what density matrix we start there will be some relaxation process which will restore $\hat{\rho}$ to the thermal equilibrium $\hat{\rho} = \hat{\rho}^T$.
- We can add damping in a phenomenological way by adding a term which will damp the density matrix to the thermal equilibrium density matrix with equilibration time T_e :

$$\dot{\hat{\rho}} = \frac{1}{i\hbar} [\hat{H}, \hat{\rho}] - \frac{\hat{\rho} - \hat{\rho}^T}{T_e},$$

the added relaxation term will have no influence on the density matrix when it is in equilibrium.

- In many cases there are TWO relaxation times T_1 and T_2 . T_1 is a damping time for population differences (described by r_3 component of the Bloch vector), it is the energy decay time. The off-diagonal components r_1 and r_2 correspond to coherences and they are only non-zero if you have two states populated with a well-defined relative phases. When the quantum mechanical system loses its memory of the phase, r_1 and r_2 components go to zero. Therefore the time T_2 is a time that describes the loss of coherence, the dephasing time. In general $T_2 < T_1$ (often by a lot).
- Using the times T_1 and T_2 we can now write the Bloch equations in a proper way:

$$\begin{aligned} \dot{r}_z &= (\boldsymbol{\omega} \times \mathbf{r})_z - \frac{r_z - r_z^T}{T_1} \\ \dot{r}_{x,y} &= (\boldsymbol{\omega} \times \mathbf{r})_{x,y} - \frac{r_{x,y} - r_{x,y}^T}{T_2} \end{aligned}$$

- The addition of phenomenological decay times does not generalize the density matrix enough to cover situations where atoms (possibly state-selected) are added or lost to a system. This situation can be covered by the addition of further terms to $\dot{\rho}$. Thus a calculation on a resonance experiment in which state-selected atoms are added to a two-level system through a tube which also permits atoms to leave (e.g. a hydrogen maser) might look like:

$$\dot{\rho} = \frac{1}{i\hbar}[H, \rho] - \begin{pmatrix} (\rho_{11} - \rho_{11T})/T_1 & \rho_{12}/T_2 \\ \rho_{21}/T_2 & (\rho_{22} - \rho_{22T})/T_1 \end{pmatrix} + R \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} - \rho/T_{\text{escape}} - \rho/T_{\text{collision}}$$

where R is the rate of addition of state-selected atoms. The last two terms express effects of atom escape from the system and of collisions (e.g. spin exchange) that can't easily be incorporated in T_1 and T_2 .

The terms representing addition or loss of atoms will not have zero trace, and consequently will not maintain $\text{Tr}(\hat{\rho}) = 1$. Physically this is reasonable for systems which gain or lose atoms; the application of the density matrix to this case shows its power to deal with complicated situations. In most applications of the above equation, one looks for a steady state solution (with $\dot{\rho} = 0$), so this does not cause problems.

- Every process which contributes to T_1 will also contribute to T_2 but there are lots of processes which only contribute to T_2 . Therefore in general T_2 is much faster because many more process contribute to it. T_1 is the time to damp population and that is a damping of $|\Psi|^2$. T_2 is due to the damping of the phase and this is more of a time of the wavefunction itself (Ψ). So if the only process that is happening is eg. spontaneous emission T_1 can be faster than T_2 (when it is defined as above). With our definition of T_1 and T_2 more proper way of comparing the times is: $\frac{T_2}{2} \leq T_1$.