Density Matrix Theory

Lectures	Tue	12:00 - 13:30	PHY 5.0.20
	Thu	10:15 - 12:00	PHY 9.1.09
Exercises	Fri	10:15 - 12:00	PHY 5.0.21

Sheet 2

1. Time evolution for a closed three level system (analytics)

Consider a three level system described by the Hamiltonian (in position representation):

$$H = \begin{pmatrix} \varepsilon_1 & b & b \\ b & \varepsilon_2 & b \\ b & b & \varepsilon_3 \end{pmatrix},$$

which you can interpret, for example, as the Hueckel Hamiltonian of a three-atomic molecule, where ε_i with $i = 1, 2, 3$ are the on-site energies of the three atoms and b describes the hopping between the atoms. Study the quantum dynamics of the system by means of the Liouville-von Neumann equation:

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

where ρ is the (single particle) density matrix for the molecule. In particular:

1. Show by explicit writing of the corresponding equiation of motions that, in general, the dynamics of the population is coupled to the one of the coherences. Moreover, show that the dynamics of population and coherences is decoupled if the density matrix is written in the energy eigenbasis.

2. Consider the homoatomic case ($\varepsilon_1 = \varepsilon_2 = \varepsilon_3$) and calculate explicitly the time evolution of the density matrix both in energy and position representation in terms of a generic initial condition: $\rho_{ij}(t = 0) = \rho^0_{ij}$

   (Hint: Every operator $\hat{\mathcal{O}}$ (including the density operator $\hat{\rho}$) has different matrix representations depending on the choice of the basis in the Hilbert space of the system. Nevertheless all representations are equivalent and connected by unitary transformation.

   $$\tilde{\mathcal{O}} = U\mathcal{O}U^\dagger$$

   Find the transformation that diagonalizes the Hamiltonian and solve the problem first in the representation in which H is diagonal.)

2. Time evolution for a closed three level system (numerics)

Consider the same problem of the first exercise. But this time look for a numerical solution to the problem. The basic idea is to discretize the time and to calculate the density matrix at time $t + \Delta t$ according to the formula:

$$\rho(t + \Delta t) = \rho(t) - \frac{i}{\hbar}[H, \rho(t)]\Delta t$$

1. Plot the populations as a function of time for different initial conditions. What happens if for example you prepare the electron on the first atom of the molecule at time $t = 0$?

2. Can you plot the results also in the energy basis?
3. What happens to the dynamics if you prepare the system in a statistical mixture in the energy basis?
4. Compare the results with the analytical ones: is the numerics acceptable?
5. What happens if you make the Δt smaller?

An example for the two-level system is on-line at:

`http://homepages.ur.de/~doa17296/fisica/Teaching/ST18_DMT/ST18_DMT.html`

Frohes Schaffen!