Tutorial sheet 6

6. Evolution equations for the statistical operator

The statistical operator $\hat{\rho}$ of a quantum-mechanical system governed by the Hermitian Hamiltonian $\hat{\mathsf{H}}(t)$ satisfies the Liouville–von Neumann equation

$$\frac{\mathrm{d}\hat{\rho}(t)}{\mathrm{d}t} = \frac{1}{\mathrm{i}\hbar}\big[\hat{\mathsf{H}}(t), \hat{\rho}(t)\big] \tag{1}$$

where $[\,\cdot\,,\,\cdot\,]$ denotes the commutator of two operators. In this exercise we derive several useful results that will be used in the lectures.

i. Schrödinger picture

Let $\hat{\mathsf{U}}(t,t_0)$ denote the unitary time-evolution operator between the times t_0 and t associated with the Hamiltonian $\hat{\mathsf{H}}(t)$, such that the state vector $|\Psi(t)\rangle$ for the system at time t is related to the state vector at t_0 by $|\Psi(t)\rangle = \hat{\mathsf{U}}(t,t_0)\,|\Psi(t_0)\rangle$.

Recall which differential equation (and with which initial condition) is fulfilled by $\hat{\mathsf{U}}(t,t_0)$. Show that $\hat{\mathsf{U}}(t,t_0)$ also relates the values of the statistical operator at t_0 and t:

$$\hat{\rho}(t) = \hat{\mathsf{U}}(t,t_0)\,\hat{\rho}(t_0)\,\hat{\mathsf{U}}(t,t_0)^\dagger. \tag{2}$$

ii. Interaction picture

Assume that the Hamiltonian is of the form $\hat{\mathsf{H}}(t) = \hat{\mathsf{H}}_0 + \hat{\mathsf{W}}(t)$ where $\hat{\mathsf{H}}_0$ is time independent. The interaction-picture representation of the statistical operator is related to its Schrödinger representation $\hat{\rho}(t)$ by

$$\hat{\rho}_{\mathrm{I}}(t) = \mathrm{e}^{\mathrm{i}\hat{\mathsf{H}}_0 t/\hbar}\,\hat{\rho}(t)\,\mathrm{e}^{-\mathrm{i}\hat{\mathsf{H}}_0 t/\hbar} \tag{3}$$

(which as you may check is consistent with the interaction-representation $|\Psi(t)\rangle_{\mathrm{I}} \equiv \mathrm{e}^{\mathrm{i}\hat{\mathsf{H}}_0 t/\hbar}\,|\Psi(t)\rangle$ of state vectors).

a) Which differential equation of the Liouville–von Neumann type is obeyed by $\hat{\rho}_{\mathrm{I}}(t)$? Compare with the equation governing the evolution of $|\Psi(t)\rangle_{\mathrm{I}}$. (*Hint:* You may want to introduce the interaction representation $\hat{\mathsf{W}}_{\mathrm{I}}(t) = \mathrm{e}^{\mathrm{i}\hat{\mathsf{H}}_0 t/\hbar}\,\hat{\mathsf{W}}(t)\,\mathrm{e}^{-\mathrm{i}\hat{\mathsf{H}}_0 t/\hbar}$.)

b) Propose a formal solution of the form (2) to the evolution equation you found in question **a)**, using an appropriate unitary operator $\hat{\mathsf{U}}_{\mathrm{I}}(t,t_0)$ which you should specify. Again, you may check the consistency with the time evolution of $|\Psi(t)\rangle_{\mathrm{I}}$.

c) Check that the usual formula involving the statistical operator to express the expectation value of an observable $\hat{\mathsf{O}}$ can also be used in interaction picture, provided one uses $\hat{\rho}_{\mathrm{I}}(t)$ and the interaction representation $\hat{\mathsf{O}}_{\mathrm{I}}(t)$ — whose expression in terms of $\hat{\mathsf{O}}$ you can probably guess by now.

iii. Instead of expressing the statistical operator with the help of the time evolution operator as in Eq. (2), one can write down a formal solution of Eq. (1) in integral form. Indeed, check that integrating the Liouville–von Neumann equation (in Schrödinger picture) between times t_0 and t leads first to

$$\hat{\rho}(t) = \hat{\rho}(t_0) + \frac{1}{\mathrm{i}\hbar}\int_{t_0}^{t}\big[\hat{\mathsf{H}}(t'), \hat{\rho}(t')\big]\,\mathrm{d}t', \tag{4}$$

and equivalently to

$$\hat{\rho}(t) = \hat{\rho}(t_0) + \frac{1}{\mathrm{i}\hbar}\int_{t_0}^{t}\big[\hat{\mathsf{H}}(t'), \hat{\rho}(t_0)\big]\,\mathrm{d}t' + \frac{1}{(\mathrm{i}\hbar)^2}\int_{t_0}^{t}\bigg\{\int_{t_0}^{t'}\Big[\hat{\mathsf{H}}(t'), \big[\hat{\mathsf{H}}(t''), \hat{\rho}(t'')\big]\Big]\,\mathrm{d}t''\bigg\}\,\mathrm{d}t'. \tag{5}$$

Of course, one can write similar relations in interaction representation.