Real Time Formalism (Schwinger-Keldysh closed time path formalism)

Before (in imaginary time – Matsubara – formalism), we took the quantum mechanical density operator to be

$$\hat{\rho}(\beta) = e^{-\beta \hat{H}} \quad \leftarrow \text{a system at equilibrium}$$

Now, choose a more general density operator:

$$\underline{\hat{\rho}(t)} = \sum_n p_n \underbrace{|\psi_n(t)\rangle\langle\psi_n(t)|}_{\substack{\text{States NOT NECESSARILY} \\ \text{E-STATES OF HAMILTONIAN}}}$$

Probability of finding QM system in state $|\psi_n\rangle$.

Note that the density operator describing the system is a function of (real) time.

n.b. ensemble average (of operator $\hat{A}$) $\langle A\rangle(t) \equiv Tr[\hat{\rho}(t)\hat{A}]$

(of course, we may choose $p_n = e^{-\beta E_n}$ so that the system is in thermal equilibrium). – for now take p_n arbitrary & independent of time.

Time evolution of $\hat{\rho}(t)$:

The time evolution of $\hat{\rho}(t)$ is governed by the von Neumann equation, the quantum mechanical analogue of the Liouville equation in classical mechanics:

$$i\hbar \frac{\partial}{\partial t}\hat{\rho} = i\hbar\frac{\partial}{\partial t}\sum_n p_n |\psi_n(t)\rangle\langle\psi_n(t)|$$

$$= \sum_n p_n \left(\underbrace{i\hbar \frac{\partial|\psi_n(t)\rangle}{\partial t}}_{\hat{H}|\psi_n(t)\rangle}\langle\psi_n(t)| + i\hbar\, |\psi_n(t)\rangle \underbrace{\frac{\partial\langle\psi_n(t)|}{\partial t}}\right)$$

$$-\langle\psi_n(t)|\hat{H}$$

$$\boxed{i\hbar\frac{\partial}{\partial t}\hat{\rho} = [\hat{H}, \hat{\rho}]} \qquad \underline{\text{von Neumann Equation}}$$

– not to be confused with the Heisenberg equation of motion, which has a minus sign.

Notice that if the Hamiltonian has no explicit time dependence,

$$\hat{\rho}(t) = \sum_n p_n |\psi_n(t)\rangle\langle\psi_n(t)| = \sum_n p_n \, e^{-i\hat{H}t} |\psi_n(0)\rangle\langle\psi_n(0)| \, e^{+i\hat{H}t}$$

$$= e^{-i\hat{H}t}\,\hat{\rho}(0)\,e^{+i\hat{H}t}, \qquad \left[\text{otherwise} \quad U(t) = T e^{-i\int dt' \hat{H}(t')}\right]$$

and if the Hamiltonian commutes with $\hat{\rho}(0)$, then

$$\hat{\rho}(t) = \hat{\rho}(0)\,\cancel{e^{-i\hat{H}t}}\,\cancel{e^{+i\hat{H}t}} = \hat{\rho}(0). \qquad \text{(can be seen from vN. eqn)}$$

the density matrix is independent of time.

TRUE when ① $\hat{\rho}(t)$ written in terms of stationary states.

② p_n's have Boltzmann distribution (thermal equil.)

If the system is not in equilibrium, move to Heisenberg representation.

$$|\psi(t)\rangle = \underbrace{e^{-i\hat{H}(t-t_0)}}_{\text{Unitary time evolution operator}} |\psi(t_0)\rangle$$

- can be written: $\hat{U}(t,t_0) = T\exp\left[-i\int_{t_0}^{t} dt'\,\hat{H}(t')\right]$

$$\hat{U}^\dagger(t,t_0) = \hat{U}(t_0,t) = \tilde{T}\exp\left[i\int_{t_0}^{t} dt'\,\hat{H}(t')\right]$$

anti-time ordering symbol

- satisfies composition rule:

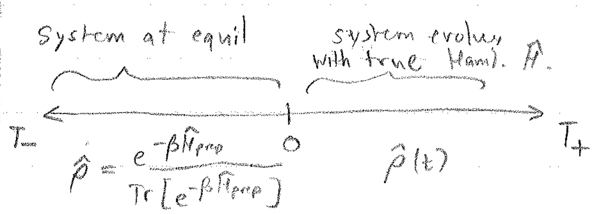
$$\hat{U}(t_3,t_2)\,\hat{U}(t_2,t_1) = \hat{U}(t_3,t_1)$$

$$\hat{U}(t_2,t_1)\,\hat{U}(t_1,t_2) = 1.$$

Setup:

Prepare the system in an equilibrium state at (inverse) temperature β at negative times, with a preparatory Hamiltonian, $\hat{H}_{prep}$.

Then, at positive times, let the system evolve with the true Hamiltonian, $\hat{H}_{true}(t)$, which may be time dependent.



$$\hat{H} = \begin{cases} \hat{H}_{prep}, & t < 0 \\ \hat{H}_{true}(t), & t > 0. \end{cases}$$

Clearly, the system will reach equilibrium by $\hat{H}_{prep}$, and we can safely describe it with a density operator, at time $t=0$, of the form

$$\hat{\rho}(0) = \frac{e^{-\beta \hat{H}_{prep}}}{Tr[e^{-\beta \hat{H}_{prep}}]} \qquad \text{[equilibrium w.r.t } \hat{H}_{prep}]$$

It will be convenient to write it in terms of time evolution operators:

$$= \frac{\hat{U}(T_- - i\beta, T_-)}{Tr[\hat{U}(T_- - i\beta, T_-)]} \qquad \text{take } T_- \ll 0. \quad (T_- \text{ large negative number})$$

Time-dependent ensemble averages (of operator $\hat{A}$)

$$\langle A \rangle(t) = Tr[\hat{\rho}(t)\hat{A}] = Tr[\hat{U}(t,0)\hat{\rho}(0)\hat{U}(0,t)\hat{A}]$$

insert $\hat{1} = U(0,T_-)\,U(T_-,0)$

$$= \frac{Tr[\hat{U}(t,0)\hat{U}(T_- - i\beta, T_-)\hat{U}(0,t)\hat{A}]}{Tr[\hat{U}(T_- - i\beta, T_-)]}$$

$$\langle A\rangle(t) = \frac{\mathrm{Tr}\Big[\overbrace{\underbrace{\hat{U}(t,0)\hat{U}(0,T_-)}_{}}^{\hat{U}(t,T_-)\ \longrightarrow\ \text{cyclic}}\ \hat{U}(T_-,0)\ \hat{U}(T_- - i\beta,\, T_-)\ \hat{U}(0,t)\,\hat{A}\Big]}{\mathrm{Tr}\big[\hat{U}(T_- - i\beta,\, T_-)\big]}$$

commute through

Insert $\mathbb{1} = \hat{U}(T_-,T_+)\hat{U}(T_+,T_-)$

$T_+ \equiv$ large positive time ($T_+ \gg 0$)

$$= \frac{\mathrm{Tr}\Big[\hat{U}(T_- - i\beta,\, T_-)\ \overbrace{\hat{U}(T_-,0)\ \hat{U}(0,t)}^{\hat{U}(T_-,t)}\ \hat{A}\ \hat{U}(t,T_-)\Big]}{\mathrm{Tr}\big[\hat{U}(T_- - i\beta,\, T_-)\big]}$$

$$= \frac{\mathrm{Tr}\Big[\hat{U}(T_- - i\beta,\, T_-)\ \hat{U}(T_-,T_+)\ \overbrace{\hat{U}(T_+,T_-)\ \hat{U}(T_-,t)}^{\hat{U}(T_+,t)}\ \hat{A}\ \hat{U}(t,T_-)\Big]}{\mathrm{Tr}\big[\hat{U}(T_- - i\beta,\, T_-)\big]}$$

$$= \frac{\mathrm{Tr}\Big[\hat{U}(T_- - i\beta,\, T_-)\ \hat{U}(T_-,T_+)\ \hat{U}(T_+,t)\ A\ \hat{U}(t,T_-)\Big]}{\mathrm{Tr}\big[\hat{U}(T_- - i\beta,\, T_-)\big]} \qquad t>0$$

Pictorially,