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1. Define the density operator

$$\hat{\rho}(t) \equiv \sum_j P_j |\Psi_j(t)\rangle\langle\Psi_j(t)|, \tag{1}$$

where P_j is the probability of finding the ensemble being in the state $|\Psi_j(t)\rangle$ at time t. Note here $\{P_j\}$ is the classical probability with mixing quantum states $\{|\Psi_j(t)\rangle\}$ in an incoherent way. Show that the density operator satisfies the Liouville–von Neumann equation,

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}(t) = [\hat{H}, \hat{\rho}(t)], \tag{2}$$

with the given Hamiltonian $\hat{H}$. Furthermore, show that density operators at different times are related by a unitary transformation. Find the unitary operator.

2. The von Neumann entropy is defined via

$$S_{\mathrm{vN}} \equiv -k_B \mathrm{Tr}(\hat{\rho}\ln\hat{\rho}), \tag{3}$$

with k_B being the Boltzmann constant. For an isolate system, when it approaches to the thermodynamic equilibrium, the entropy reaches maximum, that is

$$\delta S = 0, \tag{4}$$

and the density operator satisfies

$$\dot{\hat{\rho}} = -\frac{i}{\hbar}[\hat{H}, \hat{\rho}] = 0. \tag{5}$$

Prove that for this system,

$$\hat{\rho} = \frac{1}{\Omega}\sum_j |\psi_j\rangle\langle\psi_j|, \tag{6}$$

with $|\psi_j\rangle$ $(j = 1, 2, \cdots)$ being the eigenstates of the system Hamiltonian and Ω the total number of states. (*Hint: The condition* $\mathrm{Tr}\hat{\rho} = 1$ *may be helpful.*)