

Quantum Thermodynamics File2:Akk2Mani

Ashok Kapoor

March 10, 2022

1. Suppose I have a isolated system. Will it not be described by a time independent Hamiltonian? For an quantum system the time evolution of the density of states will be given by the standard equation.

$$i\hbar\frac{d\rho}{dt} = [H, \rho]$$

If we take ρ at time $t = 0$ to be some function of H , it will be a constant of motion. To me this appears to be an equilibrium situation. If yes, what is meant by the temperature of such state?

2. What I have written above applies to, for example, a single particle state system in an energy eigen state. And also to an assembly of **non-interacting** particles, each particle being in some energy eigen state.
3. Both the cases correspond to a pure state with definite energy eigenvalue.
4. Even if a system is not in pure state, the density matrix can be written as a sum $\sum_n p_n |E_n\rangle\langle E_n|$. This is not an equilibrium state, because the density matrix will keep evolving according to Schrodinger equation. It is not at all clear the quantum evolution of such a system can give rise to density matrix of the form that will correspond to a definite temperature.

$$\rho = \frac{e^{-\beta H}}{Z} \quad (1)$$

5. Let us look at the whole issue from a different angle. Suppose I have quantum system of several particles. Let us assume that the total Hamiltonian is independent of time. Let us assume that the probability of system being in energy state E_n has some initial value p_n . Then under quantum evolution, the probability of energy being E_n will remain constant. These probabilities will never evolve to that given by Boltzmann distribution.
6. Thus to me it seems that for a statistical system of large number of particles, it is not a correct model the system as a ensemble of particles and to assume that the Hamiltonian of the system is independent of time.

It thus seems that there are no stationary states for a real system with a large number, 10^{23} , of particles.

These comments have been posted on zero space. [Click here to go to 0space page](#)

‘Your File is renamed, [ashok.pdf → File01Mani2Akk](#), and is attached.

This discusses some of the issues raised by Ashok during our discussions on the properties of quantum systems and its relation to thermodynamics.

1. Given a density matrix, what is the meaning of temperature of the system?

Temperature has a meaning only under equilibrium conditions and it has the form

$$\hat{\rho} = \frac{\exp(-\beta\hat{H})}{\text{TrTr}(\exp(-\beta\hat{H}))} \quad (1)$$

The same is true for classical systems where we need to have the probability distribution function $\rho(q, p)$ to be given by

$$\rho(q, p) = \frac{\exp(-\beta H(q, p))}{\int dqdp \exp(-\beta H(q, p))} \quad (2)$$

Thus the system has a temperature only if it (quantum)system satisfies Eq.(?) or (classical) eq.(?).

In general, a density matrix defining a system need not be in thermal equilibrium.

An important question arises is answering the question

What does thermal equilibrium mean ?

Only if they obey eq.(ref1) or (??).

However, if a closed (isolated) system is not in thermal equilibrium, the question arises what happens to it subsequently. The energy of the system is fixed. The law of statistical mechanics states that the system attains an equilibrium state which has the maximum of

$$- \int dqdp \rho \ln(\rho(q, p)) \quad (3)$$

for the classical case and

$$- \text{Tr}(\hat{\rho} \ln(\hat{\rho})) \quad (4)$$

How this comes about is the subject of ergodic theory (needs sophisticated mathematical analysis, for both the classical and the quantum case). The time scales are important in analysing a process.

Thus in the case of classical adiabatic equation, the time scale of expansion should be larger than the time scale of thermalisation (relaxation time), so that at every stage, the system has a definite temperature, pressure etc. Here, only states which are in thermal equilibrium is being considered.

On the other hand in the case of quantum adiabatic process, consider a density matrix which is diagonal in the energy basis and is at thermal equilibrium at temperature T . When this develops quantum adiabatically by changing the Hamiltonian slowly, the probability of a particular state does not change. However energy changes and so the system is out of thermal equilibrium. So in this case, we assume the time scale of thermalization to be larger than the time scale at which the quantum adiabatic theorem is valid.

Finally, all the four postulates of Callen are for thermally equilibrium states only. They are therefore valid for both classical and quantum systems.

Not every state, quantum or classical need satisfy these postulates (non-equilibrium systems) usually referred to as open systems (classical or quantum)