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A new look at the quantum Liouville theorem

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Abstract

We clarify certain confusions in the literature of the density operator in quantum mechanics, and demonstrate that the quantum Liouville theorem has the same form in both the Schrodinger and the Heisenberg pictures. Our starting point is to treat the density operator as an observable which has its specific time dependence in each of the two pictures. It is further shown that such a formulation will provide the exact correspondence between classical and quantum statistical mechanics with the Liouville theorem being interpreted as a conservation law, which is derivable from the equation of motion only in the quantum case.

Keywords: Density operator, Quantum Liouville Theorem, Pictures of time evolution

1. Introduction

As is well known, the density operator defined as the outer product of the state vectors is a very useful concept in quantum statistical mechanics, especially in treating systems of mixed states [1]. Although density matrix formulation is only an alternative approach which is equivalent to that from using state vectors in conventional quantum mechanics [2], the recent proposition by Weinberg [3] to replace state vectors by density operators in a new formulation of quantum mechanics can lead to a future central role played by these operators. Thus it will be significant for a clarification of certain confusing issues with these operators sometimes arise in the literature. In particular, the time evolution of these operators via the quantum Liouville theorem has been ambiguous in terms of the picture of time evolution as well as the total/partial time derivatives of these operators. For example, while claims can be found from various online website that the time evolution of the density matrix holds only in the Schrodinger or interaction picture [4]; others claim that such a Liouville theorem also holds in the Heisenberg picture but with the wrong sign as that in the Heisenberg equation, and is due to the fact that the density operator is not an observable [2, 4-5].

In this communication, we shall provide a consistent formulation showing that the same form of the Liouville theorem actually holds in both the Schrodinger and Heisenberg pictures, providing an exact correspondence between classical and quantum statistical mechanics, with both cases originated from the law of conservation of microstates/probability. Our results are consistent with some previous works which had this clarified via an assertion for the vanishing of the total derivative of the density operator in the Heisenberg picture [6, 7], except that we provide a rigorous justification for this via a clarification on the unitary transformation of operators between the different pictures for the time evolution in quantum mechanics.

2. Brief review on classical statistical mechanics

For a system of N classical particles, we have the phase space density $\rho(x_i, p_i, t)$ defined as the number of microstates per phase space volume satisfying the following equation:

$$\begin{aligned} \frac{d\rho}{dt} &= \sum_{i=1}^{3N} \left(\frac{\partial \rho}{\partial x_i} \frac{\partial x_i}{\partial t} + \frac{\partial \rho}{\partial p_i} \frac{\partial p_i}{\partial t} \right) + \frac{\partial \rho}{\partial t} \\ &= \sum_{i=1}^{3N} \left(\frac{\partial \rho}{\partial x_i} \frac{\partial H}{\partial p_i} - \frac{\partial \rho}{\partial p_i} \frac{\partial H}{\partial x_i} \right) + \frac{\partial \rho}{\partial t} \\ &= \{\rho, H\}_{PB} + \frac{\partial \rho}{\partial t} \end{aligned} \quad (1)$$

where we have used the Hamilton canonical equations and the definition of the Poisson bracket. Hence, conservation of the number of phase space points (microstates):

$$\frac{d\rho}{dt} = 0 \Rightarrow \frac{\partial \rho}{\partial t} = \{H, \rho\}_{PB} \quad (2)$$

The classical Liouville theorem established in (2) simply follows from the continuity equation for the phase space current density: $\vec{\nabla} \cdot (\rho \vec{v}) + \frac{\partial \rho}{\partial t} = 0$, where the phase space “velocity” is defined as :

$\vec{v} = (v_{x_1}, \dots, v_{x_{3N}}; v_{p_1}, \dots, v_{p_{3N}})$ with $v_{x_i} = \frac{dx_i}{dt}$ and $v_{p_i} = \frac{dp_i}{dt}$, respectively; and the divergence is a $6N$ dimensional operator. It is important to emphasize the significance in the difference between the total and partial time derivatives in the statement of this theorem in (1) and (2), and that such conservation law is imposed on ρ rather than derived from the equation of motion.

3. Quantum statistical mechanics

For simplicity, we shall consider only the density operator for pure states as the results can be generalized in a straightforward manner to mixed states. Thus we have:

$$\hat{\rho} = |\psi\rangle\langle\psi| \quad (3)$$

In our formalism, we shall regard $\hat{\rho}$ to correspond to an observable (i.e. dynamic variable) since this just yields the probability density within a certain representation (e.g. $\langle x|\hat{\rho}|x\rangle = |\psi(x)|^2$) which can be measured in experiments such as those involving the interference of particles. Hence its time derivative ($\partial\hat{\rho}/\partial t$) is also a dynamic variable. This is in contrast to some of the treatments in the literature [2, 4, 5]. We shall show that the operator defined in (3) will have its time evolution correctly governed by the appropriate equations of motion (i.e. the Schrodinger and the Heisenberg equation, respectively) in each of the two pictures. The important thing to note is that all operators must transform from one picture to another via the same universal unitary transformation. We shall demonstrate the consistency and the classical correspondence of the quantum Liouville equation in both these pictures in the following. As for notation, we shall denote quantities in the Heisenberg picture with a subscript ‘H’ and those in the Schrodinger picture without any subscript for simplicity.

(i) Schrodinger picture

From the time dependent Schrodinger equation:

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = \hat{H} |\psi\rangle \quad (4)$$

and its conjugate:

$$i\hbar \frac{\partial}{\partial t} \langle\psi| = -\langle\psi| \hat{H} \quad (5)$$

we thus obtain:

$$\begin{aligned} i\hbar \frac{\partial \hat{\rho}}{\partial t} &= i\hbar \frac{\partial |\psi\rangle}{\partial t} \langle\psi| + |\psi\rangle i\hbar \frac{\partial \langle\psi|}{\partial t} \\ &= \hat{H} |\psi\rangle \langle\psi| - |\psi\rangle \langle\psi| \hat{H} \\ &= \hat{H} \hat{\rho} - \hat{\rho} \hat{H} \\ &= [\hat{H}, \hat{\rho}] \end{aligned} \quad (6)$$

Hence the quantum Liouville theorem or von Neuman equation obtained in (6) is directly correlated to the classical result in (2) via the “Dirac quantization Rule”:

$$\{H, \rho\}_{PB} \rightarrow \frac{1}{i\hbar} [\hat{H}, \hat{\rho}] \quad (7)$$

Let us provide the following three remarks on the above results:

(a) Although we used to regard only the quantum state but not the observable to vary in time in the Schrodinger picture, the density operator is an exception since it is an operator defined as a function (outer product) of the quantum states.

(b) The distinction between the partial and the total time derivatives in (4)-(6) must be consistent, since if one confuses the former with the latter, one will be misled when a representation (e.g. the x representation) is adopted. This has indeed occurred in the literature [8].

(c) In the position representation, the result in (6) leads back to the continuity equation which expresses conservation of probability in wave mechanics.

(ii) Heisenberg picture

To transform from the Schrodinger to the Heisenberg picture, we shall impose the following unitary transformation:

$$|\psi\rangle \rightarrow |\psi\rangle_H = U^\dagger |\psi\rangle \quad (8)$$

$$\hat{A} \rightarrow \hat{A}_H = U^\dagger \hat{A} U \quad (9)$$

so that the expectation value is invariant:

$${}_H \langle \psi | \hat{A}_H | \psi \rangle_H = \langle \psi | \hat{A} | \psi \rangle. \quad (10)$$

For conservative time-independent Hamiltonian, one simply has:

$$U = e^{-iHt/\hbar} \quad (11)$$

A very important consequence of (9) which has sometimes been overlooked in the literature is the fact that the (partial) time derivative of an operator in the Heisenberg picture is not the same as the ‘‘Heisenberg operator’’ of the same time derivative of this operator in the Schrodinger picture, that is:

$$\frac{\partial \hat{A}_H}{\partial t} \neq \left(\frac{\partial \hat{A}}{\partial t} \right)_H \quad (12)$$

This is obvious if we explicitly use (9) into (12) and obtain:

$$\frac{\partial}{\partial t} (U^\dagger \hat{A} U) \neq U^\dagger \left(\frac{\partial \hat{A}}{\partial t} \right) U \quad (13)$$

We believe that the confusion of the result in (12) is the origin of some of the ambiguous conclusions about the quantum Liouville theorem in the literature as elaborated in the following. Thus, we have in this picture the state vectors being constant in time but operators evolve in time according to the Heisenberg equation:

$$i\hbar \frac{\partial \hat{A}_H}{\partial t} = [\hat{A}_H, \hat{H}_H] + i\hbar \left(\frac{\partial \hat{A}}{\partial t} \right)_H \quad (14)$$

We would like to provide another three remarks on Eq. (14):

(d) Without adopting any representation, there is no difference between total and partial time derivatives in either (4) or (14), since the state vector or the operator can only be function of time.

(e) Since we have already kept using partial derivative in the Schrodinger picture as explained in point (b) above, we naturally arrived at (14) with all partial derivatives.

(f) However, it is customary to rewrite the LHS of (14) as a total derivative.

This is done only for notation purpose to distinguish the two derivatives on the two sides of the equation as pointed out in Eq. (12), which is very helpful especially when the subscript ‘‘H’’ is removed from Eq. (14) [6, 7]. Thus we rewrite (14) in the following form:

$$i\hbar\left(\frac{d\hat{A}}{dt}\right)_H = [\hat{A}_H, \hat{H}_H] + i\hbar\left(\frac{\partial\hat{A}}{\partial t}\right)_H \quad (15)$$

where we simply have the notation:

$$\left(\frac{d\hat{A}}{dt}\right)_H \equiv \frac{\partial\hat{A}_H}{\partial t} = \frac{\partial}{\partial t}(U^\dagger\hat{A}U) \quad (16)$$

Another motivation to introduce the total derivative notation in (16) is to ensure (15) to go back to the correct corresponding classical result in Hamiltonian mechanics (cf Eq. (1)) via the procedure in Eq. (7). Note that a common mistake in the literature is to confuse the term $\left(\frac{\partial\hat{A}}{\partial t}\right)_H$ in (14) with

$\frac{\partial\hat{A}_H}{\partial t}$ (see, e.g., Refs. [6], [7], [9]). We shall see below that by requiring the total time derivative of the density operator in (16) to vanish, one will lead to a formalism which is both consistent with the Schrodinger picture and in correspondence with classical statistical mechanics. Since we have regarded the density operator to correspond to an observable, we expect (15) to hold for it as well (with $[\hat{\rho}_H, \hat{H}_H] \equiv [\hat{\rho}, \hat{H}]_H$):

$$i\hbar\left(\frac{d\hat{\rho}}{dt}\right)_H = [\hat{\rho}, \hat{H}]_H + i\hbar\left(\frac{\partial\hat{\rho}}{\partial t}\right)_H \quad (17)$$

Since Eq. (6) expresses an operator equation in Schrodinger picture, a unitary transformation making use of the time evolution operator (cf. Eqs. (9) and (11)) will validate it to hold also in the Heisenberg picture:

$$i\hbar\left(\frac{\partial\hat{\rho}}{\partial t}\right)_H = [\hat{H}, \hat{\rho}]_H \quad (18)$$

Thus, the combination of Eqs. (17) and (18) leads to the vanishing of the total derivative:

$$i\hbar\left(\frac{d\hat{\rho}}{dt}\right)_H = 0 \quad (19)$$

The result in (19) is consistent with those in Refs. [6] and [7] and is seen to be exactly the quantum correspondence of the classical conservation of phase space current as expressed in Eq. (2). Note that this is a good example illustrating the result in (12) since in this case one will have

$$\frac{\partial\hat{\rho}_H}{\partial t} = \frac{\partial}{\partial t}(|\psi\rangle_H\langle\psi|_H) = 0 \neq \left(\frac{\partial\hat{\rho}}{\partial t}\right)_H = \frac{1}{i\hbar}[\hat{H}, \hat{\rho}]_H \quad (20)$$

a consequence of the well-known fact that $|\psi\rangle_H = U^\dagger|\psi\rangle = |\psi(0)\rangle = \text{constant}$ in time.

We believe this is the origin of most of the confusion in the literature about the quantum Liouville theorem such as those claiming that it has the “wrong sign” as the Heisenberg equation of motion, or $\hat{\rho}$ is not an observable [4, 5]. Hence the density operator first introduced in Schrodinger picture

via Eq. (3) is really special in Heisenberg picture for it satisfies a conservation law. Note that in the Schrodinger picture, a corresponding result as in (19) also holds with the density operator being replaced by its expectation value [8]:

$$i\hbar \left(\frac{d\langle \hat{\rho} \rangle}{dt} \right)_s = 0 \quad (21)$$

We remark that while (2) is a consequence of the conservation of “phase space current” in classical mechanics, the uncertainty principle will restrict (19) and (21) to imply the conservation of probability current in either the position or the momentum space, when either one of these representations is adopted. In addition, the quantum Liouville theorem in (19) and (21) are consequences from the equation of motion (the Schrodinger or Heisenberg equation) and no separate imposition of a conservation law is required for their validity to hold. This is in analogy with the well-known mathematical derivation of conservation of probability from the Schrodinger equation in wave mechanics [10]. On the other hand, the Liouville theorem in Eq. (2) in the classical case is not a consequence of the equation of motion, and must be imposed as an independent conservation law for the time evolution of the system in phase space.

4. Conclusion

Since the first recognition by von Neumann [1] and Dirac [11] of the correspondence between the density operator and the phase space density via the Liouville theorem in both quantum and classical statistical mechanics, respectively, confusion on this issue has emerged in the literature from time to time [4, 5, 8, 9]. From the above analysis, it is seen that the Liouville theorem has the same form both in classical and in quantum mechanics, and in the latter, it also has the same operator form in both the Schrodinger and Heisenberg pictures. Most of the confusion arises due to the overlooking of the result pointed out in our Eqs. (12) and (20). Thus the conclusion that the density operator in the Heisenberg picture satisfies the “Heisenberg equation with the wrong sign” [2, 4, 5] is misleading. Rather, this operator satisfies exactly the Heisenberg equation just like any other observable, except that it is a rare case with explicit time dependence in the Schrodinger picture, which becomes constant in the Heisenberg picture upon the unitary transformation given in Eq. (9).

Hence we conclude that statements such as (i) the Liouville theorem is only valid in the Schrodinger or interaction picture; or (ii) the Liouville theorem also applies in the Heisenberg picture but with the wrong sign with reference to the Heisenberg equation, are simply erroneous. The quantum Liouville theorem is just an expression of conservation of probability current with the classical phase space density replaced by the density operator in quantum mechanics.

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