

# Of quantum mechanical pictures

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## 1 Introduction

In quantum mechanics, a pure state of a system is described by a vector  $|\Psi\rangle$  of an appropriate Hilbert space  $\mathfrak{H}$ , and its time evolution is governed by the Schrödinger equation, a first-order homogeneous linear differential equation:

$$\frac{d|\Psi\rangle}{dt} = A|\Psi\rangle. \quad (1)$$

For closed systems, the linear operator  $A$  is anti-Hermitian, and can therefore be written as

$$A = \frac{H}{i\hbar}, \quad (2)$$

where  $H$  is Hermitian and turns out to be the Hamiltonian of the system. In the following we shall refer to this situation as unitary evolution.

However, for open systems, the Hamiltonian of the system (if it has any sense at all)<sup>1</sup> is non-Hermitian, and hence we cannot assume anything on the behaviour of the operator  $A$  with respect to Hermitian conjugation. What we

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<sup>1</sup>E.g. in a well-established method for theoretical treatment of open systems in state-vector formalism, the Monte Carlo wave-function method, the time propagation is described by a non-Hermitian Hamiltonian operator interrupted by random quantum jumps.

do assume is that  $A$  is time-independent, a *very important restriction*, which is adopted throughout in this treatise.

Generally, the state of the system will not be pure and hence it has to be described by a density operator  $\rho$ . A density operator can always be written as a convex combination of state vector dyads:

$$\rho = \sum_l p_l |\Psi_l\rangle \langle \Psi_l|, \quad p_l > 0, \quad \sum_l p_l = 1. \quad (3)$$

The time evolution of the density operator is governed by the quantum Master equation

$$\frac{d\rho}{dt} = 2\Re \{A\rho\} + J\rho J^\dagger - \frac{1}{2} [J^\dagger J, \rho]_+ =: 2\Re \{A'\rho\} + J\rho J^\dagger, \quad A' := A - \frac{J^\dagger J}{2}.^2 \quad (4)$$

We are introducing the notation for the real and imaginary parts of operators:

$$\Re \{M\} = \frac{M + M^\dagger}{2}, \quad \Im \{M\} = \frac{M - M^\dagger}{2i} \quad (5)$$

If  $O$  is a Hermitian operator on  $\mathfrak{H}$ , it is called a quantum mechanical observable, and its expectation value in a pure state  $|\Psi\rangle$  is

$$\langle O \rangle = \langle \Psi | O | \Psi \rangle, \quad (6)$$

and it is a real number. If the state is mixed

$$\langle O \rangle = \text{Tr} \{O\rho\}. \quad (7)$$

## 1.1 Transformations

Quantum mechanical pictures in a general way can be introduced as follows: Let us consider the operator

$$T \equiv e^{Bt}, \quad (8)$$

where  $B$  is an arbitrary linear operator and the transformation defined as

$$|\Psi\rangle =: T |\Psi_T\rangle \Leftrightarrow |\Psi_T\rangle := T^{-1} |\Psi\rangle. \quad (9)$$

From this and Eq. (3) follows that a density operator under this transformation is transformed as

$$\rho_T = T^{-1} \rho (T^\dagger)^{-1}, \quad (10)$$

so that it remains Hermitian, but in general it does not have unit trace. Similarly, the transformed state vector (9) is in general not a normalized one.

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<sup>2</sup>The most general form of a Master equation is of course with several Lindblad (jump) operators  $J$ , but from the point of view of the transformations treated here this would not make a difference.

Physics has to remain unaffected by the transformation, so we enforce that quantum expectation values remain the same: Hence, the observables have to be transformed as well:

$$\langle \Psi_T | O_T | \Psi_T \rangle = \langle O_T \rangle := \langle O \rangle = \langle \Psi | O | \Psi \rangle = \langle \Psi_T | T^\dagger O T | \Psi_T \rangle, \quad (11)$$

whence the transformed observable reads

$$O_T = T^\dagger O T, \quad (12)$$

and it is also a Hermitian operator.

## 1.2 Transformed equations of motion

From Eqs. (1) and (9) the equation of motion for the transformed state vector is

$$\frac{d|\Psi_T\rangle}{dt} = (T^{-1}AT - B)|\Psi_T\rangle = (A^T - B)|\Psi_T\rangle =: \mathcal{A}^T |\Psi_T\rangle. \quad (13)$$

Here we have introduced another type of operator transformation, which we denote by superscript. If  $C$  is an operator, we therefore have two kinds of transformed operator

$$C_T = T^\dagger C T, \text{ and} \quad (14a)$$

$$C^T = T^{-1} C T. \quad (14b)$$

One has to be careful, however, that when it comes to density operators, the transformation (10) is different from that of other operators. The physical content of the density operator is of course also different: in spite of being an operator, it describes the *state* of the system.

The transformed Master equation reads:

$$\frac{d\rho_T}{dt} = 2\Re \{ \mathcal{A}^T \rho_T \} + J^T \rho_T (J^T)^\dagger. \quad (15)$$

The equation of motion for the transformed observables reads:

$$\frac{dO_T}{dt} = 2\Re \{ O_T B \} + \left( \frac{dO}{dt} \right)_T. \quad (16)$$

This equation is known as the Heisenberg equation.

## 1.3 Unitary transformation

When the generator of the transformation  $B$  is anti-Hermitian, the transformation operator  $T$  is unitary. In this case the two forms (14) of transforming operators coincide. The transformed state vector remains normalized to one, and the transformed density operator remains normalized to unit trace.

## 2 Interaction picture

Let us assume that operator  $A$  is of the form

$$A := A^{(1)} + A^{(2)}, \quad (17)$$

and the generator of the transformation operator

$$B := A^{(1)}. \quad (18)$$

In this case the generator of the system's dynamics in Eqs. (13) and (15) simplifies to

$$\mathcal{A}^T = (A^{(2)})^T, \quad (19)$$

while the Heisenberg equation reads

$$\frac{dO_T}{dt} = 2\Re \{O_T A^{(1)}\} + \text{“} . \quad (20)$$

That is, as a result of the transformation, time propagation gets split between the state of the system and system observables: the part defined by  $A^{(2)}$  pertaining to the former, and  $A^{(1)}$  to the latter. For this to be advantageous, it is desirable that we are in some sense able to “solve” this latter part, so that we can easily deal with expressions like  $e^{A^{(1)}t}$ .

### 2.1 Special case: Heisenberg picture

From the general interaction picture defined above, the Heisenberg picture is obtained in the case when  $A^{(2)} := 0$ , that is

$$B = A. \quad (21)$$

This makes that in this picture state vectors do not evolve

$$|\Psi_H(t)\rangle = |\Psi_H(0)\rangle = |\Psi(0)\rangle, \quad (22)$$

time propagation being completely reflected upon observables. The Heisenberg equation in the language of the Hamiltonian reads:

$$\frac{dO_H}{dt} = \frac{2}{\hbar} \Im \{O_H H\} + \text{“} = \frac{i}{\hbar} (H^\dagger O_H - O_H H) + \text{“} \xrightarrow{\text{unitary}} \frac{i}{\hbar} [H, O_H] + \text{“}. \quad (23)$$

If we consider the energy of the system as an observable, in general it is only in the unitary case that we have

$$H_H = H. \quad (\text{In unitary case only}) \quad (24)$$

Otherwise, the only thing we can say is

$$H^H = H, \quad (\text{Generally true}) \quad (25)$$

which is the reason why in Eq. (23) we find the operator  $H$  pure and simple.

Furthermore, it is worth noting that if the Hamiltonian has the form  $H = H^{(1)} + H^{(2)}$ , though it is true that  $H^H = H$ , it is in general *not* true that  $(H^{(i)})^H = H^{(i)}$ . The latter holds only in the case when  $[H^{(1)}, H^{(2)}] = 0$  because in this case the transformation operator gets factorised:

$$T = \left( e^{H^{(1)}} e^{H^{(2)}} \right)^{\frac{i}{\hbar}}. \quad (26)$$

However, it is always true that  $(H^{(i)})^H$  and  $H^{(i)}$  have the same *algebraic form*, if each one is written with operators of the corresponding picture, since in operator products, the identity  $T \cdot T^{-1}$  can always be inserted between the factors.