Emphasizing the Role of Time in Quantum Dynamics

J. Jeener

Université Libre de Bruxelles (CP-232)
Campus Plaine, B-1050 Brussels, Belgium

Contents

I. Introduction **35**

II. Bases and Representations **36**
1. Single basis, single date 36
2. Single basis, two dates (or more) 37
3. Two bases, two dates (or more) 37

III. Time Derivatives As Seen From Different Bases **38**

IV. Quantum Dynamics As Seen From Different Bases **39**
1. Laboratory frame 39
2. Rotating frame 40
3. Interaction representation 41

V. Acknowledgments **41**

VI. References **42**

I. Introduction

Richard Ernst begins his Nobel Lecture entitled "Nuclear Magnetic Resonance Fourier Transform Spectroscopy" (1) with the remark that NMR is one of the first fields in which quantum theory and experiments have been discussed with time (and not energy or frequency) as the essential explicit variable, eventually leading to the general concept of "coherent spectroscopy." Again and again, when teaching the elementary aspects of quantum dynamics and pulsed NMR, I felt dissatisfied with the traditional way of handling the time-related variables and transformations, and I progressively developed an alternative presentation which leads to the same conclusions in a somewhat different way. It is a real pleasure to present these ideas in this issue of the *Bulletin of Magnetic Resonance* as a tribute to a very good friend, Richard Ernst.

One customary weakness is to use the same name ("time"), and similar typographic symbols, for dates and for durations (i.e. time intervals). Of course, this does not disturb or confuse the experts, but it is inconvenient and misleading for beginners, and intolerable if one tries to get systematic help from a symbolic manipulation program. Solving this problem is just a matter of care in the choice of words, symbols and notation.

Another, more subtle, traditional weakness has to do with the comparison or combination of quantum objects defined at different dates, as involved in the definition of time-derivatives for instance. To illustrate this point, let us examine the seemingly obvious notion of a constant ket, taking as a prototype one of the kets forming the basis b in current use in ket space. If we should be taking the ideas of "rotating frame" or "toggling frame" literally, we would be using different bases in ket space associated with the different "frames", and these bases would be moving with respect to each other. Clearly, a ket which appears as immobile or constant with respect to one of these bases will, in general, appear as time-dependent with respect to other bases. "Absolute rest" is not a valid concept in quantum state space any more than in ordinary configuration space. With this situation in mind, the traditional presentation of quantum dynamics appears as strongly tied to a particular choice of basis in ket space, a choice on which attention is usually not drawn explicitly. If we want to avoid this limitation, for the sake of generality and uniformity, or in order to retain full freedom in the final choice of basis for the evaluation of traces, we should mention the reference basis explicitly, whenever relevant, and formulate quantum dynamics in such a way that the reference basis can be changed at will, while keeping the same abstract quantum objects for the description of the physical situation under investigation. As we shall see, this does not require any major change in notation or logic, and tends to make the quantum engineering more systematic and transparent [see, for instance, ref. (2)].

Consequences of dropping the tacit notion of absolute rest are that, for instance,

(a) all kets will carry a date tag and operations on kets like linear combination or scalar product will be meaningful *only* if the kets involved are all defined at the same date,

(b) changing the date tag(s) of a quantum object will appear as an important transformation in itself,

(c) time-derivatives of quantum objects will be labelled by the basis in which they are evaluated,

(d) c-number objects, like matrix elements or traces, have a date-dependence which is not related to any particular choice of basis, hence providing a convenient tool for linking objects with different basis labels.

The ideas and techniques which are discussed in the present paper for the "ket-bra-operator" presentation of quantum mechanics can be extended to the "Liouville" presentation in a particularly simple way if Liouville space objects are introduced, which are the *direct* counterparts of kets, bras and operators [see, for instance, ref. (3)]. The resulting limitation to superkets and superbras which do not change the date, hence to superoperators which involve two dates at most, does not seem to be a hindrance, at least for NMR applications.

For simplicity, the discussion will be limited to non-relativistic problems which can be described in terms of discrete bases in ket space. No attempt will be made towards more generality.

II. Bases and Representations

For clarity in the present paper, we shall write explicitly, for each quantum object, all the arguments which are date tags, and no other. If other arguments were necessary, the typography should clearly separate date tag(s) from other arguments.

As a starting point, we choose a basis b in ket space, which is a collection of kets $|b_i(t)\rangle$ which, at any date t, satisfies the orthonormality condition

$$\Big\langle b_j(t)\Big|b_k(t)\Big\rangle = \delta_{j,k} \tag{1}$$

and the closure relation

$$\sum_i \Big|b_i(t)\Big\rangle\Big\langle b_i(t)\Big| = 1, \tag{2}$$

where 1 denotes the unit or identity operator (note that this operator is defined without reference to any specific basis or date, hence a date tag would be irrelevant).

1. Single basis, single date

As long as a single date t is involved, no deviation from the traditional procedures is necessary: Any ket $|\psi(t)\rangle$ can be expressed ("represented") as a linear combination of the kets of the basis $\{|b_i(t)\rangle\}$ by the usual multiplication from the left with the closure relation eqn. 2

$$\Big|\psi(t)\Big\rangle = 1\Big|\psi(t)\Big\rangle = \sum_i \Big|b_i(t)\Big\rangle\Big\langle b_i(t)\Big|\psi(t)\Big\rangle. \tag{3}$$

This procedure is easily extended to linear operators $A(t)$ involving a single date, which are defined by the linear relation between $|\psi(t)\rangle$ and $|\varphi(t)\rangle = A(t)|\psi(t)\rangle$ for any $|\psi(t)\rangle$. A representation of the operator $A(t)$ in terms of the single-date level-shift basis $\{|b_j(t)\rangle\langle b_k(t)|\}$ is easily obtained by multiplication of $A(t)$ by the closure relation eqn. 2 from both right *and* left

$$A(t) = \sum_{j,k} \Big|b_j(t)\Big\rangle\Big\langle b_k(t)\Big|\Big\langle b_j(t)\Big|A(t)\Big|b_k(t)\Big\rangle. \tag{4}$$

2. Single basis, two dates (or more)

As a first example involving two dates, let us consider the operator $P_{b,i}(t_1, t_0) = |b_i(t_1)\rangle\langle b_i(t_0)|$, which has the obvious property $P_{b,i}(t_1, t_0)|b_i(t_0)\rangle = |b_i(t_1)\rangle$ whenever $|b_i(t_0)\rangle$ is normalized. The action of this operator to its right on a ket $|\alpha\rangle$ is defined only if the date tag of this ket is t_0, and the result is then the ket $|\beta\rangle = P_{b,i}(t_1, t_0)|\alpha(t_0)\rangle$ with date tag t_1. Of course, $|\beta(t_1)\rangle$ may also depend implicitly on t_0.

Conversely, the action of $P_{b,i}(t_1, t_0)$ to its left on a bra is defined only if the date tag of the bra is t_1, and the result is then a bra with date tag t_0. Summarizing, the operator $P_{b,i}(t_1, t_0)$ has date tags t_1 on its left and t_0 on its right, as indicated explicitly by the typography (t_1, t_0) of the pair of date tags.

Clearly, such date-changing operators can be added together (only) if they have the same pair of date tags, and they can be multiplied together (only) if the sides which are in contact have the same date tag. For instance, one can easily verify that $P_{b,i}(t_2, t_0) = P_{b,i}(t_2, t_1)P_{b,i}(t_1, t_0)$.

The ket $|\psi(t)\rangle$ will be called immobile *as seen from basis* b if all its projections on this basis are independent of the date t, hence

$$\begin{aligned}\Big|\psi(t)\Big\rangle &= \sum_i \Big|b_i(t)\Big\rangle\Big\langle b_i(t)\Big|\psi(t)\Big\rangle \\ &= \sum_i \Big|b_i(t)\Big\rangle\Big\langle b_i(t_0)\Big|\psi(t_0)\Big\rangle \\ &= U_b(t, t_0)\Big|\psi(t_o)\Big\rangle,\end{aligned} \tag{5}$$

where t_0 is some fixed date, and the unitary date displacement operator associated with basis b,

$$U_b(t, t_0) = \sum_i \Big|b_i(t)\Big\rangle\Big\langle b_i(t_0)\Big|, \tag{6}$$

has all the usual properties of evolution operators, including the group property for connected date pairs

$$U_b(t_2, t_0) = U_b(t_2, t_1)U_b(t_1, t_0) \tag{7}$$

and the relations

$$\begin{aligned}&U_b(t, t) = 1 \qquad \text{and} \\ &\Big(U_b(t, t_0)\Big)^\dagger = \Big(U_b(t, t_0)\Big)^{-1} = U_b(t_0, t).\end{aligned} \tag{8}$$

Note that the definition of the inverse, as the solution of the equation $\Big(U_b(t, t_0)\Big)^{-1}U_b(t, t_0) = 1$ with a unit operator involving a single date, implies that the inverse has the date tags t on the right and t_0 on the left, hence the unit operator has the tacit date tag t_0.

The operator $B(t)$ involving a single date will be called immobile *as seen from basis* b if all its matrix elements $\langle b_j(t)|B(t)|b_k(t)\rangle$ in this basis are independent of t. Such an operator can be expressed for any date t in terms of the operator at a fixed date t_0 and the characteristic evolution operator $U_b(t_0, t)$ of basis b as

$$B(t) = U_b(t, t_0)B(t_0)U_b(t_0, t). \tag{9}$$

After introducing the explicit notion of date-changing operator, in contrast to operators involving a single date, it is worth stressing that "taking the trace" is a valid operation only when applied to operators which do not change the date, for instance $\mathrm{Tr}[A(t)]$. Of course, A may be expressed as a product involving a number of date-changing operators, but this product itself must have the same date tag on either side.

3. Two bases, two dates (or more)

Let us now consider a second basis $\{|c_i(t)\rangle\}$ with characteristic evolution operator $U_c(t, t_0)$. At any single date t, basis c is related to basis b by the unitary transformation $W_{cb}(t)$, such that, for any i,

$$\Big|c_i(t)\Big\rangle = W_{cb}(t)\Big|b_i(t)\Big\rangle, \tag{10}$$

where

$$W_{cb}(t) = \sum_k \Big|c_k(t)\Big\rangle\Big\langle b_k(t)\Big| \tag{11}$$

has the usual properties

$$W_{bb}(t) = 1$$

and

$$\Big(W_{cb}(t)\Big)^\dagger = \Big(W_{cb}(t)\Big)^{-1} = W_{bc}(t). \tag{12}$$

Of course, basis kets are immobile as seen from their own basis, so that we can use eqn. 5 to obtain the relations $|c_k(t)\rangle = U_c(t, t_0)|c_k(t_0)\rangle$ and $\langle b_k(t)| = \langle b_k(t_0)|U_b(t_0, t)$, which we can insert in eqn. 11 to derive the useful transformation rules

$$U_c(t,t_0) = W_{cb}(t)U_b(t,t_0)W_{bc}(t_0)$$

and

$$W_{cb}(t) = U_c(t,t_0)W_{cb}(t_0)U_b(t_0,t). \tag{13}$$

If more than two bases are involved, (11) immediately leads to the relation

$$W_{dc}(t)W_{cb}(t) = W_{db}(t). \tag{14}$$

Consider now the particular case of a basis c such that all its basis kets $|c_i(t)\rangle$ are immobile with respect to basis b, hence $|c_i(t)\rangle = U_b(t,t_0)|c_i(t_0)\rangle$ for all i. Combining this with the definition eqn. 5 for $U_c(t,t_0)$, we conclude that $U_b(t,t_0) = U_c(t,t_0)$. Hence, two bases which are immobile with respect to each other have exactly the same characteristic evolution operator.

III. Time Derivatives As Seen From Different Bases

In the present perspective, the naive definition of the time derivative of an arbitrary ket (not necessarily mobile or immobile with respect to any specified basis) as the limit of $[|\varphi(t+\Delta t)\rangle - |\varphi(t)\rangle]/\Delta t$ for $\Delta t \to 0$ has to be supplemented with a procedure for comparing (subtracting) kets defined at *different* dates. With basis b chosen as reference, a natural way out of this problem is to interpret $|\varphi(t)\rangle$ in the above formula as the ket $U_b(t+\Delta t,t)|\varphi(t)\rangle$ which would be obtained at date $(t+\Delta t)$ if the ket $|\varphi(t)\rangle$ remained immobile *as seen from basis* b for the duration from t to $(t+\Delta t)$. With this procedure, the time derivative of a ket as seen from basis b is given by {using eqns. 2 and 6}

$$\begin{aligned}
&\left(\frac{\partial}{\partial t}\right)_b \big|\varphi(t)\big\rangle \\
&= \lim_{\Delta t\to 0}\Big[\big|\varphi(t+\Delta t)\big\rangle - U_b(t+\Delta t,t)\big|\varphi(t)\big\rangle\Big]\Big/\Delta t \\
&= \lim_{\Delta t\to 0}\Big[\sum_i \big|b_i(t+\Delta t)\big\rangle\big\langle b_i(t+\Delta t)\big|\varphi(t+\Delta t)\big\rangle \\
&\quad - \sum_i \big|b_i(t+\Delta t)\big\rangle\big\langle b_i(t)\big|\varphi(t)\big\rangle\Big]\Big/\Delta t \\
&= \sum_i \big|b_i(t)\big\rangle \frac{\partial}{\partial t}\big\langle b_i(t)\big|\varphi(t)\big\rangle,
\end{aligned} \tag{15}$$

where the time derivative of the ket has to be labelled by the relevant basis whereas the time derivatives of c-number quantities do not have such labels because they do not depend upon the choice of basis. If we multiply the first and the last terms of eqn. 15 by $\langle b_k(t)|$ from the left, and sum over i using eqn. 1, we obtain $\langle b_k(t)|\left\{\left(\frac{\partial}{\partial t}\right)_b|\varphi(t)\rangle\right\} = \frac{\partial}{\partial t}\langle b_k(t)|\varphi(t)\rangle$, hence the k-th component of the time-derivative is the time derivative of the k-th component, provided that components and time derivative refer to the same basis.

Similar definitions can be given for the time derivatives of the other types of quantum objects with respect to any specified basis [see, for instance, ref. (2)]. For instance,

$$\left(\frac{\partial}{\partial t}\right)_b A(t) = \sum_{i,k}\big|b_i(t)\big\rangle\big\langle b_k(t)\big|\frac{\partial}{\partial t}\big\langle b_i(t)\big|A(t)\big|b_k(t)\big\rangle. \tag{16}$$

Pursuing the discussion of the relations between two bases b and c, which started with eqns. 10-13, it is convenient to define an additional operator $D_{cb}(t)$ such that

$$i\hbar\left(\frac{\partial}{\partial t}\right)_b W_{cb}(t) = D_{cb}(t)W_{cb}(t),$$

hence

$$D_{cb}(t) = i\hbar\left(\frac{\partial W_{cb}(t)}{\partial t}\right)_b W_{cb}^{\dagger}(t). \tag{17}$$

$D_{cb}(t)$ has the dimension of energy, and is Hermitian because $W_{cb}(t)$ is unitary. Taking the time derivative of both sides of eqn. 10 with respect to basis b (note that basis kets are immobile with respect to their own basis) we obtain

$$\begin{aligned}
i\hbar\left(\frac{\partial}{\partial t}\right)_b\big|c_i(t)\big\rangle &= i\hbar\left(\frac{\partial W_{cb}(t)\big|b_i(t)\big\rangle}{\partial t}\right)_b \\
&= i\hbar\left(\frac{\partial W_{cb}(t)}{\partial t}\right)_b\big|b_i(t)\big\rangle = D_{cb}(t)\big|c_i(t)\big\rangle,
\end{aligned} \tag{18}$$

which leads directly to simple expressions of the relation between time derivatives with respect to two different bases, for instance

$$i\hbar\left(\frac{\partial}{\partial t}\right)_c\big|\psi(t)\big\rangle = i\hbar\left(\frac{\partial}{\partial t}\right)_b\big|\psi(t)\big\rangle - D_{cb}(t)\big|\psi(t)\big\rangle,$$

$$i\hbar\left(\frac{\partial}{\partial t}\right)_c A(t) = i\hbar\left(\frac{\partial}{\partial t}\right)_b A(t) - \Big[D_{cb}(t), A(t)\Big]. \tag{19}$$

Permuting the roles of the bases, and using eqns. 12, 14, 17 and 19 in the perspective of multiple bases, one can easily verify that

$$D_{bc}(t) = -D_{cb}(t)$$

and (20)

$$D_{db}(t) = D_{dc}(t) + D_{cb}(t).$$

IV. Quantum Dynamics As Seen From Different Bases

1. Laboratory frame

We choose basis b as the conventional reference basis in which the equation of motion for the density operator $\rho(t)$, which describes the state of the physical system, is the usual von Neumann equation

$$i\hbar\left(\frac{\partial}{\partial t}\right)_b \rho(t) = \Big[H(t), \rho(t)\Big], \tag{21}$$

where the Hermitian operator $H(t)$ is the Hamiltonian of the system. We shall assume, as usual, that the Hamiltonian and all other relevant observables of the system are well known in terms of their action on the basis kets of the reference basis b. In general, basis b and the "basic" observables are introduced, according to the standard quantization rules, starting from classical quantities defined in a particular classical frame of reference (called "laboratory frame" in the NMR literature). If this frame is inertial, then $H(t)$ is both the generator of motion with respect to basis b, as shown by eqn. 21, and the energy observable suitable for discussing thermodynamics in this classical frame.

Combining eqns. 19 and 21, we see immediately that $\rho(t)$ is immobile in any basis d such that $D_{db}(t) = H(t)$, hence, using eqn. 9, we have

$$\rho(t) = U_d(t,t_0)\rho(t_0)U_d(t_0,t). \tag{22}$$

The characteristic evolution operator $U_d(t,t_0)$ of basis d can be evaluated by solving its equation of motion

$$i\hbar\left(\frac{\partial}{\partial t}\right)_b U_d(t,t_0) = H(t)U_d(t,t_0) \tag{23}$$

directly, with the initial condition $U_d(t_0,t_0) = 1$, or by solving the equation of motion for the unitary transformation $W_{db}(t)$,

$$i\hbar\left(\frac{\partial}{\partial t}\right)_b W_{db}(t) = H(t)W_{db}(t), \tag{24}$$

with a suitable unitary initial condition and using eqn. 13.

A useful step towards approximate solutions of eqns. 23 or 24 for short delays is to reformulate the problem as an equivalent integral equation. For instance, we can use the version of eqn. 15 for operators to cast eqn. 24 under the form

$$\begin{aligned} W_{db}(t+\Delta t) = {} & U_b(t+\Delta t,t)W_{db}(t)U_b(t,t+\Delta t) \\ & + \Delta t\; H(t)W_{db}(t) \end{aligned} \tag{25}$$

in the limit of $\Delta t \to 0$. This process of infinitesimal date change can be iterated, leading to the simple integral equation version of eqn. 24, including the initial condition:

$$\begin{aligned} W_{db}(t) = {} & U_b(t,t_0)W_{db}(t_0)U_b(t_0,t) \\ & + \frac{1}{i\hbar}\int_{t_0}^{t} dt_1 U_b(t,t_1)H(t_1)W_{db}(t_1)U_b(t_1,t). \end{aligned} \tag{26}$$

Eqn. 26 can be used recursively to derive the usual formal series expansion

$$\begin{aligned} W_{db}(t) = {} & U_b(t,t_0)W_{db}(t_0)U_b(t_0,t) \\ & + \frac{1}{i\hbar}\int_{t_0}^{t} dt_1 U_b(t,t_1)H(t_1)\times \\ & U_b(t_1,t_0)W_{db}(t_0)U_b(t_0,t) \\ & + \left(\frac{1}{i\hbar}\right)^2 \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 U_b(t,t_1)H(t_1)\times \\ & U_b(t_1,t_2)H(t_2)U_b(t_2,t_0)W_{db}(t_0)U_b(t_0,t) + \ldots \end{aligned} \tag{27}$$

In the case of $U_d(t,t_0)$, similar calculations lead from eqn. 23 to

$$\begin{aligned} U_d(t,t_0) = {} & U_b(t,t_0) \\ & + \frac{1}{i\hbar}\int_{t_0}^{t} dt_1 U_b(t,t_1)H(t_1)U_b(t_1,t_0) \\ & + \left(\frac{1}{i\hbar}\right)^2 \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 U_b(t,t_1)H(t_1)\times \\ & U_b(t_1,t_2)H(t_2)U_b(t_2,t_0) + \ldots \end{aligned} \tag{28}$$

The analogous expression for $\rho(t)$ in terms of $\rho(t_0)$ involves nested commutators with the Hamiltonian taken at different dates, also with U_b operators bridging the "gaps" between different date tags.

As usual, the difficulties involved in deriving a compact version of these formal series expansions depend crucially on the commutation properties of $H(t)$ with itself taken at different dates. In the present formalism, the simple case is when

$$\Big[H(t_1), U_b(t_1,t_2)H(t_2)U_b(t_2,t_1)\Big] = 0 \tag{29}$$

for any pair of dates t_1 and t_2 ranging from t_0 to t (note that the above commutator is an operator with a single date tag), which implies, for example, that

$$U_d(t,t_0) = \exp\left\{\int_{t_0}^{t} dt_1 U_b(t,t_1)H(t_1)U_b(t_1,t_0)\right\}, \tag{30}$$

where no "time ordering" is involved so that the integral can be evaluated first and the exponential taken as a final step. Comparison of eqn. 29 with eqn. 9 shows that the commutator in eqn. 29 is zero whenever $H(t)$ is immobile with respect to basis b, as expected. Clearly, the issue about commutation depends upon the basis (b in the present case) in which the differential equation is formulated.

We are now ready to evaluate the average value $\langle A(t)\rangle$ of any observable $A(t)$ for any initial state $\rho(t_0)$ of the system as

$$\begin{aligned}\langle A(t)\rangle &= \mathrm{Tr}\Big\{A(t)\rho(t)\Big\} \\ &= \mathrm{Tr}\Big\{A(t)U_d(t,t_0)\rho(t_0)U_d(t_0,t)\Big\}.\end{aligned} \tag{31}$$

In the "laboratory frame" presentation of the calculations, all operators will be expressed in terms of the corresponding "basic" observables, so that bases suitable for the evaluation of the trace will presumably be basis b itself, or bases which are immobile with respect to basis b.

2. Rotating frame

Discussions about quantum dynamics are often greatly simplified if the Hamiltonian can be written as the sum of two Hermitian operators,

$$H(t) = H_0(t) + \Big\{H(t) - H_0(t)\Big\} \tag{32}$$

such that $H_0(t)$ alone would generate a simple motion, and $\{H(t) - H_0(t)\}$ is (much) smaller than $H_0(t)$. The standard technique for using eqn. 32 is known in the NMR literature under the name of "going over to the rotating frame" with the understanding that this "rotating frame" moves with respect to the "laboratory frame" according to the dynamics generated by $H_0(t)$.

In the present context, we shall take this idea literally as meaning that quantum dynamics should be examined with reference to a basis c which moves with respect to basis b in such a way that $D_{cb}(t) = H_0(t)$, hence the transformation operator from basis b to basis c is a solution of (see eqn. 24)

$$i\hbar\left(\frac{\partial}{\partial t}\right)_b W_{cb}(t) = H_0(t)W_{cb}(t) \tag{33}$$

with a suitable unitary initial condition, hence eqn. 21, the equation of motion for $\rho(t)$, can be written as

$$i\hbar\left(\frac{\partial}{\partial t}\right)_c \rho(t) = \left[\Big\{H(t) - H_0(t)\Big\}, \rho(t)\right]. \tag{34}$$

This confirms the expectation that, as seen from basis c, the motion of $\rho(t)$ is governed by the "small" generator of motion $\{H(t) - H_0(t)\}$. This "slow" motion is best described by the transformation operator from basis c to basis d (see eqn. 22), which is a solution of the equation of motion

$$i\hbar\left(\frac{\partial}{\partial t}\right)_c W_{dc}(t) = \Big\{H(t) - H_0(t)\Big\}W_{dc}(t) \tag{35}$$

with a suitable unitary initial condition. When $W_{dc}(t)$ and $W_{cb}(t)$ are known, the evolution operator $U_d(t,t_0)$ for $\rho(t)$ is directly given by eqns. 13 and 14.

Solving eqns. 34 or 35 still presents the practical problem that the time-derivatives are "as seen from basis c." A simple way out of this problem is to express all the relevant operators in terms of a new set of basic operators which are immobile with respect to basis c. For each original basic operator $B(t)$, immobile with respect to the original basis b, we can introduce a corresponding member $B^{[cb]}(t)$ of the new set as

$$B^{[cb]}(t) = \Big\{W_{cb}(t)B(t)W_{bc}(t)\Big\} = \Big\{U_c(t,t_0)B(t_0)U_c(t_0,t)\Big\}, \tag{36}$$

hence

$$B(t) = W_{bc}(t)\Big\{W_{cb}(t)B(t)W_{bc}(t)\Big\}W_{cb}(t) = W_{bc}(t)B^{[cb]}(t)W_{cb}(t). \tag{37}$$

Pursuing in the same direction, we shall find that the final evaluation of the trace in eqn. 31 will also be simplified by the use of basis c or some basis immobile with respect to basis c.

The procedure indicated in this section is perfectly practical and has the major advantages of being the *exact* analogue of the general idea of one same experiment (involving the system under investigation, "external actions," and measuring instruments) being examined and discussed by various observers who try to choose the most convenient point of view. Of course, this procedure has the minor drawback of an unusual typography: time derivatives are indexed by the relevant basis, a new set of basic operators is introduced for each new basis,...

If we are willing to drop the major advantage of physical clarity mentioned above, we can very easily translate the many-bases procedure into the conventional single-basis "interaction representation" technique.

3. Interaction representation

In the rotating frame procedure outlined above, the "original" operators (density operator, Hamiltonian, observables, evolution operator,...) are discussed with reference to the "not-original" basis c. If we apply the transformation $W_{bc}(t)$ to all these quantum objects, basis c is transformed into basis b, each operator is transformed into its $^{[bc]}$ transform (note the rule for date changing operators),

$$A^{[bc]}(t) = W_{bc}(t)A(t)W_{cb}(t), \quad \Big\{C^{[cb]}(t)\Big\}^{[bc]} = C(t), \quad K^{[bc]}(t,t_0) = W_{bc}(t)K(t,t_0)W_{cb}(t_0), \tag{38}$$

time derivatives with respect to basis c are transformed into time derivatives with respect to basis b, hence eqn. 34 is transformed into an equation of motion for $\rho^{[bc]}(t)$, formulated in basis b,

$$i\hbar\left(\frac{\partial}{\partial t}\right)_b \rho^{[bc]}(t) = \left[\Big\{H^{[bc]}(t) - H_0^{[bc]}(t)\Big\}, \rho^{[bc]}(t)\right]. \tag{39}$$

The solution of eqn. 39 can be written as

$$\rho^{[bc]}(t) = U_d^{[bc]}(t,t_0)\rho^{[bc]}(t_0)U_d^{[bc]}(t_0,t) \tag{40}$$

where

$$U_d^{[bc]}(t,t_0) = W_{dc}^{[bc]}(t)U_b(t,t_0)W_{cd}^{[bc]}(t_0) \tag{41}$$

and

$$i\hbar\left(\frac{\partial}{\partial t}\right)_b W_{dc}^{[bc]}(t) = \Big\{H^{[bc]}(t) - H_0^{[bc]}(t)\Big\}W_{dc}^{[bc]}(t). \tag{42}$$

Of course, average values can be evaluated from the transformed versions of the relevant operators:

$$\Big\langle A(t)\Big\rangle = \mathrm{Tr}\Big\{A(t)\rho(t)\Big\} = \mathrm{Tr}\Big\{A^{[bc]}(t)\rho^{[bc]}(t)\Big\}. \tag{43}$$

As far as practical calculations are concerned, including the introduction of suitable approximations, the interaction representation method described by eqns. 32-33 and eqns. 38-43, and the rotating frame method described by eqns. 32-37, are equivalent because they only differ by minor details of notation, as shown above. The purpose of the rather clumsy notation used in this paragraph is to clarify the relation between the quantum objects which describe the same physical object in the two methods, hence helping to combine the more intuitive visualisation provided by the rotating frame with the traditional convenience of interaction representations.

V. Acknowledgments

Discussions with P. Broekaert and F. Henin helped to clarify many aspects of the present text.

This work was supported, in part, by "Loterie Nationale" and FRSM, and by "Communauté Française de Belgique" (contrat ARC 91/96-149).

VI. References

[1]see, for instance, R. R. Ernst, *Bull. Magn. Reson.* **16**, 5-32 (1994).

[2]J. Jeener and F. Henin, *Phys. Rev.* **A34**, 4897 (1986), Appendix D. In this reference, (D33) must be corrected by replacing 1 by $U_b(t, t_0)$.

[3]J. Jeener, *Adv. Magn. Reson.* **10**, 1 (1982).