Towards a Quantum Molecular Measurement Theory:

Stern-Gerlach Thought Experiments at the Interface of Hilbert and Real Spaces

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Artículo dedicado a Fernando Zuloaga, in memoriam.
Gran amigo y científico que tomó la ruta del recuerdo
un poco antes que nosotros. OT.

Abstract
A model is presented to describe measurements in quantum mechanics that are energy conserving and based on a consistent use of the linear superposition principle. Measurements contain two aspects: recording and reading. Recording elicits full coherent interaction of the object quantum system with the quantum measuring apparatus (QMA). Stern-Gerlach experiments are analyzed and used to introduce practical aspects of the recording/reading processes. Reading subsequent to a recording is performed with special QMA endowed with local properties that are included in the present scheme as special boundary conditions. Two classes of local reading are defined: reading-in-amplitude (RIA) and reading-in-intensity (RII). The latter corresponds to populations or local counts. The former preserves quantum mechanical nature and serves to prepare quantum states from local sources. The existing mathematical structure of quantum mechanics is used without introducing the standard measurement and probabilistic postulates. A local RII, expressed as a final (irreversible) counting process, yields results in agreement with the standard statistical interpretation of quantum mechanics.
1. Introduction

Recently, a quantum theory of chemical processes has been developed on the basis of quantum molecular states (QMSs)[1-6]. These QMSs diagonalize the molecular Coulomb Hamiltonian, yielding a quantum molecular basis set (QMB) of products of diabatic electronic, vibration, rotation and translation wave functions; for detailed analyses and more recent definition see refs.[4;5;7;8]. The physical state of a given system corresponds to specific linear superpositions in the QMB. Induced by external fields or by Jahn-Teller like electron-phonon operators [5;6;9] chemical reactions are identified by changes of the coefficients in the given QMB; this requirement collides with the standard collapse of the wave function of von Neumann quantum measurement theory [10;11] as it has been discussed by Fidder and Tapia [12]. Now, all the coefficients entering in the definition of the corresponding quantum state must be determined. Furthermore, chemical processes take place in real space while the chemical change takes place in Hilbert space [3;7;13]. For this reason, a well-defined procedure is required to relate Hilbert space evolution to what experimentalists could observe in a laboratory [5]. A measurement theory compatible with the present situation is elaborated here starting from an earlier formulation [12] ( for more recent work along these lines see[7;12]. Simple Stern-Gerlach experiments are used for discussing the main issues (Cf. Section 2).

The separation of the global quantum system into two asymptotic non-interacting subsystems is shared with the standard theory of measurement [11]. Here, the representation of a measurement process is separated in two steps [12]: First, a quantum recording of the interaction or reading in amplitude (RIA); this procedure is adapted for preparations of new states. The second is a reading of such a recording; here, two possibilities are considered: 1) Local elements are introduced to observe quantum counting phenomena; this is reading in intensity (RII); 2) Other experiments are performed to prepare new quantum amplitudes or recover those imprinted. Local features make part of measuring apparatuses (shape and
position in real space) which will be expressed in the reading step via physical changes operated on the quantum amplitudes and phases.

The paper is organized as follows. Section 2 contains the theoretical aspects and formalism for the special case of separable interaction operators [12]. In section 3, Stern-Gerlach (SG) experiments are used to illustrate the reading of recordings. The RII and RIA processes are defined here. Section 4 closes the paper and includes a short discussion of situations where a recovering of coherent imprinting is possible.

2. Theoretical scheme

The concept of quantum state is fundamental to quantum mechanics [14;15]. Hilbert spaces are used to expand quantum states with the help of the linear superposition principle [10;14;15]. A quantum state is hence the set of complex coefficients, amplitudes and phases that are gathered in a row vector, all referring to a given basis set (the elements of which are collected as a column vector). The molecular basis model based on the generalized electronic approach fulfils this property.

In the standard theory of measurement, information on quantum states is collected by applying von Neumann’s reduction (projection) postulate [10]. Here the dominating view is that a single measurement event reports only the eigenvalue of a single element in the linear superposition, and simultaneously, the system collapses into the corresponding eigenstate. The systems are considered as objects having a particular set of quantum numbers. However, it has always been apparent that by performing this latter procedure information on the relative phases becomes irretrievable. This problem has been with us ever since the early days of quantum mechanics, Schrödinger criticized this type of measurement theory [16], for which he distilled the Cat Paradox. The recent summary given by Laloë shows that no solution to this problem has yet been found [17].

The time evolution of the isolated compound system is always driven by the time dependent Schrödinger equation; i.e. quantum mechanics from within [18]. As discussed by
Zeh [11], the subsystems are initially independent, and after interaction they can be treated as separate again. This condition defines a measuring device as being independent from the measured system. The choice of the apparatus depends of course on the type of system to be measured.

2.1 Quantum states

The following is just a reminder to fix the notation and notions that might differ from the standard ones. A quantum state $|\psi\rangle$ is represented by a set of well-defined complex coefficients or co-ordinates in a given basis $\{|s_n\rangle\}$ of a Hilbert space. As usual [11], the symbol $|s_n\rangle$ represents an eigenstate of the operator $S$. This latter belongs to a complete set of commuting hermitean operators, and we use a collective $n$-label for the eigenvalue $s_n$ to identify a basis state; the Coulomb Hamiltonian operator in the molecular base is one example of this type of situation [4;5]. The set of all quantum states becomes a set of complex numbers arranged as a row vector, $(<s_1|\phi>, ..., <s_n|\phi>, ...)$; the set of all possible quantum states form a linear vector space. The set of linear combinations defines then a simple dual space not to be mixed up with the (bra) dual conjugate space [14]. In the simple dual space, a quantum state is characterized by the row-vector,

$$|\psi\rangle = (C_1, ..., C_n, ...) \ [|s_1\rangle, ..., |s_n\rangle, ...] = C \cdot |s\rangle = \sum_n C_n \ |s_n\rangle$$

(1)

$|s\rangle$ represents the column vector $[|s_1\rangle, ..., |s_n\rangle, ...]$.

The eigenstates of commuting hermitian operators provide a basis, fixed in time, that is used to represent a quantum state in Hilbert space in the sense that typically a physical system does not “reside” in any one of them. The quantum state having zero amplitudes for all but one component, say $(0, ..., 0, <s_k|\phi>, 0, ...)$ stands for the $k$-th proper state of the operator $S$ in the simple dual space. Therefore, a general quantum state is always a coherent state. Changing the phase of one component in a coherent state gives another coherent quantum state; such a change must be the result of a quantum interaction.
2.2. Recording quantum states

The recording aspect of measurement is represented as usual by an interaction between two quantum subsystems with total Hamiltonian \( H \).

\[
H = H_S + H_D + H_{S,D} = H_0 + H_{S,D}
\]  

(2)

\( H_S \) defines the object system (S) under investigation and \( H_D \) characterizes the detector (D). \( H_{S,D}(t) \) is a time dependent interaction operator that in units of \( \hbar/2\pi = 1 \) is given as:

\[
H_{S,D}(t) = \exp(\imath H_0 t)H_{S,D}\exp(-\imath H_0 t)
\]  

(3)

In the model retained here, the time independent operator is written as:

\[
H_{S,D} = (1/2)V_{S(D)} + (1/2)V_{D(S)}.
\]  

(4)

The operators \( V_{S(D)} \) and \( V_{D(S)} \) are formally equal, of course, although \( V_{S(D)} \) is interpreted as a field operator connecting the system S to the detector D, and vice versa. For example, in the dipole-dipole approximation the operator \( V_{S(D)} \) stands for the scalar product \( -\mu_S \cdot E_D \), and \( V_{D(S)} \) is analogously defined as \( -\mu_D \cdot E_S \); for the case of a Stern-Gerlach experiment, the field \( E \) stands for a magnetic field and \( \mu \) is a magnetic dipole operator. Note that the basis set should contain all quantum states of the complete system and, consequently, only transitions among quantum states are forming the kernel used to construct the response functions associated with the subsystems.

Following Zeh [11] the direct product of the basis sets of the two subsystems, \( \{j^S\} \otimes \{k^D\} = \{j^S > k^D\} \), is taken to represent quantum states. Before measurement, say time \( t_0 \), one assumes that the object and detector systems are prepared in the quantum states \( |\phi(S)\rangle \) and \( |\phi(D)\rangle \), respectively; this is equivalent to give a set of initial amplitudes for both subsystems. In Hilbert space, the state prepared at \( t_0 \) is the product \( |\psi(t_0)\rangle = |\phi(D)\rangle |\phi(S)\rangle \). Taking \( \hbar/2\pi = 1 \), the time ordering operator \( T \) [19] allows writing the time evolution of the global system [11] \( |\psi(t)\rangle \) as:
\[ \left| \Psi(t_f) \right> = U(t_f, t_o) \left| \Phi_{(D)} \right> \left| \Phi_{(S)} \right> = I_r \{ \exp \left[ -\int_{t_0}^{t_f} dt' H_{S+D}(t') \right] \} \left| \Phi_{(D)} \right> \left| \Phi_{(S)} \right> = \] 

\[ T \{ \exp \left[ -\int_{t_0}^{t_f} dt' H_{S+D}(t') \right] \} \sum_j \sum_k a_j b_k \left| j \right>_S \left| k \right>_D > = \] 

\[ \sum_j \sum_j' \sum_k \sum_k' a_j(t_0) b_k(t_0) U_{jj'}^{kk'}(t_f, t_o) \left| j \right>_S \left| k \right>_D > \] 

\[ (5) \]

The initial conditions are \( U_{jj'}^{kk'}(t_o, t_o) = \delta_{jj'} \delta_{kk'} \).

The point now is to rearrange the last term in eq. (5) to make appear the initial base \( \left| j \right>_S \left| k \right>_D > \). In doing so, comparisons between initial and final states can easily be done. The completeness of the basis permits a recasting of the four dummy indexes and the expression (5) can be rewritten as

\[ \left| \Psi(t_f) \right> = \sum_j \sum_k \left( \sum_j' \sum_k' a_j b_k U_{jj'}^{kk'} (t_f, t_o) \right) \left| j \right>_S \left| k \right>_D > = \sum_j \sum_k a_j(t_f) b_k(t_f) \left| j \right>_S \left| k \right>_D > \] 

\[ (6) \]

The result can be seen as a rotation of the state vector provoked by interactions (the base states are kept fixed). This result is rigorous.

The separability hypothesis makes a detector capable of performing measurements on the object system, because before and after the quantum interaction the detector and object systems should not appear entangled. Observe that the spectra of the measuring apparatus must overlap the spectra of the measured system, totally or in part. Another fundamental hypothesis, valid for any measurement theory, is that spontaneous emission is a negligible phenomenon. Thus, a quantum that is used to change the state from \( k \) to \( k' \) in the detector comes from a transition \( j \) to \( j' \) in the measured system; a perfect measuring device must respond to all possible transitions in the measured system. In this case, an imprint of the measured system is to be found in the measuring device.

The full interaction produces changes in quantum states as time progresses, reflected as just numerical changes in the complex coefficients:

\[ \{ a_j b_k \} = \{ a_j(t_0) b_k(t_0) \} \{ a'_j b'_{k'} \} = \{ a_j(t_f) b_k(t_f) \}. \]
In the standard measurement theory, the matrix elements $U$ are obtained by applying the von Neumann operator, defined by Zeh as: $U(\text{vN})_{jj'}^{kk'} = \delta_{jj'} U_{jj'}^{kk'}$ [11]. The idea behind this latter equation is that the object system is put into a stationary state (actually a base state) by the measurement and remains there henceforth. As a consequence, it states that consecutive measurements of the same state return the same eigenvalue. This hypothesis is not retained in our approach. On the contrary, what can be measured in our approach is the set characterizing the transitions between the base states (stationary states), e.g., Balmer’s series of the hydrogen atom spectra, not even one line can be represented with one eigenvalue.

It is apparent that the simplicity reflected by the change $\{a_j b_k\} \rightarrow \{a'_j b'_k\}$ is due to basis completeness. The problem now is to show whether this transformation actually allows us to define a measurement process that, while retaining the unitary time evolution of the whole system, would permit a definition of wave functions for both the measuring apparatus and for the measured system. The interaction pattern induced by the measured object wave function is registered, as it were, in the resulting recording $\{b_k(t)\}$. While the von Neumann operator puts the object system in a basis state, the present model in contrast puts this system in a new well-defined linear superposition. The set of relative phases is conserved.

The final result elicited by the relation (6) can be written in a self-evident manner as

$$|\psi(t)\rangle - |\psi(t_0)\rangle = \sum_j \sum_k \{a_j(t) b_k(t)\} |j^S\rangle |k^D\rangle - \sum_j \sum_k \{a_j(t_0) b_k(t_0)\} |j^S\rangle |k^D\rangle$$

(7)

This is an exact result. Let us work out now a simple example (in the spirit of the linear response approach). The matrix elements of the evolution operator can be cast in terms of the dipole-dipole approximation:

$$U_{jj'}^{kk'}(t,t_0) = \delta_{jj'} \delta_{kk'} - (i) \int_{t_0}^t dt' \{ (1/2)D_{kk'}(t') E_{jj'}^S(t') + (1/2)E_{kk'}^D(t') S_{jj'}(t') \} + \ldots$$

(8)

$S_{jj'}(t)$ and $D_{kk'}(t)$ are the matrix elements of the transition moment operators, while $E_{kk'}^D(t)$ and $E_{jj'}^S(t)$ are the matrix elements of the field operators; all operators are in the interaction
representation. The matrix elements \( D_{kk'}(t) \) are products of time independent matrix elements \( D_{kk'}(t) = \langle k | \mu D | k' \rangle \) and phase factor \( \exp(i(E_k - E_{k'})t) \), with an analogous expression for \( S_{jj'}(t) \).

The correlation function \( F(t, t_o) \) is defined as:

\[
C(t, t_o) = \langle \psi(t_o) | (\psi(t) - \psi(t_o)) \rangle = \langle \psi(t_o) | \psi(t) \rangle - 1
\]  

Calculating this quantum overlap function with the initial quantum state, one gets a sum of two amplitudes, named below as \( C(D[S]) \) (i.e. a complex number related to changes in the detector quantum state after interaction with the system) and \( C(S[D]) \) (i.e. a complex number related to changes in the system wave function after interaction with the detector). For the particular model, the amplitudes \( C(D[S]) \) and \( C(S[D]) \) are defined to first order by equations (10) and (11),

\[
C(D[S]) = \langle \phi_{(D)} | D[S] \rangle = (-i/2) \sum_k \Sigma_{k'} b_k^*(t_o) b_{k'} (\sum_j \Sigma_{j'} a_{j'}^* \frac{e^{i t} E_{jj'} S(t')} D_{kk'}(t')) = \sum_k b_k^*(t_o) b_k'(t_f) \tag{10}
\]

This equation shows that the object wave function is imprinted in the \( b_{k'} \) coefficients. The new wave function for the measured system reads:

\[
C(S[D]) = \langle \phi_{(S)} | S[D] \rangle = (-i/2) \sum_j \Sigma_k a_j^* \sum_{k'} a_{j'} (\sum_k \Sigma_{k'} b_{k'}^* \frac{e^{i t'} E_{kk'} S(t')} D_{kk'}(t')) = \sum_j a_j^*(t_o) a_{j'}(t_f) \tag{11}
\]

The measuring device put the imprint on the wave function via the final coefficient \( a_{j'} \). Equation (10) and (11) are valid after time \( t_f \), which is the time when the interaction is completed. Note that the time integral contains the term \( \exp\{i(E_j^S - E_{j'}^S + E_k^D - E_{k'}^D) \tau' \} \). This factor ensures energy conservation. Under resonance conditions, namely, \( (E_j^S - E_{j'}^S + E_k^D - E_{k'}^D) = 0 \), the contributions from the integral increase proportional to the interaction time interval, \( t_f - t_o \). For those combinations of levels that are far off resonance, the integrand oscillates too fast leading to zero contributions.

After all allowed interactions have occurred or, alternatively an interaction pattern is properly defined, a separation of \( \{a'_j \} \) into the sets \( \{a'_j \} \) and \( \{b'_{k'} \} \) is the natural result.
The sets of coefficients characterize the quantum state of the respective subsystems. This follows from the structure of equation (10) and (11). This result agrees with the cluster decomposition hypothesis commonly used in quantum field theory [19]. One define the functions |D[S]> and |S[D]> after the time lapse \( t_f - t_o \) by the new set of amplitudes

\[
|D[S]> = \sum_k (-i/2) \int_{t_0}^{t_f} dt' \left( \sum_j \sum_{j'} a_j^* a_{j'} E_{jj'}^S(t') \right) (\sum_k b_k D_{kk'}(t')) |k D> = \sum_k b'_k |k D> (12)
\]

\[
|S[D]> = \sum_j (-i/2) \int_{t_0}^{t_f} dt' \left( \sum_k \sum_{k'} b_k^* b_{k'} E_{k'k}^D(t') \right) (\sum_{j'} a_{j'} S_{jj'}(t')) |j S> = \sum_j a'_j |j S> (13)
\]

The detector term (Cf. D[S]) represents the recording on the measuring apparatus of the interaction with the measured system. The detector contains now all allowed transitions produced by the fields of the object system and nothing else. In fact, as eq.(12) shows, it contains the complete imprint of the object wave function as prepared before interaction via the terms \( \sum_j \sum_{j'} a_j^* a_{j'} E_{jj'}^S(t') \). The changes produced by interactions with the system have no intrinsic randomness. Moreover, each one of the \( b'_k \) terms embodies the interactions with the incoming S-system state; this is a holographic type of interaction.

The object system, after interaction, has imprinted (see S[D]) the measuring device wave function via the corresponding terms, \( \sum_k \sum_{k'} b_k^* b_{k'} E_{kk'}^D(t') \). This is the term that modulates the object wave function after interaction. Here, again, everything is under control. At this stage, where one considers one system wave function, there are no random effects related to the interaction within this model.

The quantum amplitudes in Hilbert space, obtained from eq.(5) involve states ranging over the complete energy space. Now, if we want to come back to real space-time, energy conservation is to be imposed thereby eliminating those amplitudes on base states that cannot be “populated” with the available energy. The constraint is introduced in the next section. Note, however, that the amplitudes are modified in Hilbert space where thermodynamics arguments do not apply.
2.3. Energy conservation

The present model can be made energy conserving. In an energy basis, each basis element $|j^S\rangle|k^D\rangle$ is asymptotically related to the energy label $E_j^S + E_k^D$, and for the set $\{a_j b_k\}$ the energy of the combined state before interaction is $E(\{a_j b_k\})$ taken as equal to the expectation value of $H_o$. After the systems become asymptotic again the energy $E(\{a'_j b'_k\})$ is the expectation value of $H_o$ over the wave functions given by the eqs.(12) and (13) recast in terms of the final amplitudes $(\{a'_j b'_k\})$. For the global system, energy is conserved (unitary evolution). The following two relationships hold for the energy partitioning: $\Delta E_S = \sum_j (f(a'_j) - f(a_j))E_j^S$ and $\Delta E_D = \sum_k (f(b'_k) - f(b_k))E_k^D$, where $f(b_k)$, for instance, is $|b_k|^2$. These deltas represent the change in energy undergone by each subsystem after the interaction. The total energy change is $\Delta E_S + \Delta E_D = 0$. As a result of the measuring interactions, the changes in the measured system are correlated to the changes in the recording apparatus. What really matters, in so far as measuring is concerned, is the energy balance: $\Delta E_S + \Delta E_D = 0$. If there were no energy reshuffling among subsystem states, there would be no measurable effect.

Total linear momentum is also conserved for the present model. Thus, even if the energy “reshuffling” is such that no energy exchange can be detected, the linear momenta of the measuring and measured systems may change while conserving the total momentum. Elastic scattering is a prototype for such exchanges.

In conclusion to this section, in view of the initial conditions imposed to the system, it is apparent that a measuring of one subsystem by another is possible after they have interacted. The problem now is to amplify the effects by using other layers of measuring devices giving signals on the laboratory level. We will discuss some aspects to this problem below.
3. Measuring a wave function

The wave function is a linear superposition projected in configuration space. It is a coherent state in Hilbert space. The recording process was examined above. To complete a measurement, reading the recorded wave function is required.

In our case, equation (12) and (13) must be examined. Observe that they are linear superpositions resulting from interactions reflecting a past unitary evolution.

One of the problems is to know whether or not irreversibility makes an integral part of the measuring process when reading these quantum recordings. Moreover, a mechanism has to be defined to make contact with the statistical interpretation as a sort of internal check. To examine these and other issues, let us take as a model Stern-Gerlach apparatuses that are used to modulate (change) the quantum state of a system having a spin $S=1/2$ and study in more detail measurement in a quantum setting.

3.1. Stern-Gerlach experiments

Let us consider the simplest case illustrated in Figure 1. The wave function is a product of space-time and spin components. From a laboratory frame, the origin of the quantum system frame can be seen as if it were an inertial frame in uniform motion. In a SG experiment, energy is exchanged in space-time interactions at SG-z. There, a magnetic field gradient is used to impose a particular direction to the impulsion onto eigenstates of the spin system. For $S=1/2$ systems, the spin part of the quantum state is given by scalar products:

$$ (a_1 \ a_2) \ [l+> \ l->] = a_1 \ l+> + a_2 \ l->. $$

(14)

Standard normalization is assumed: $|a_1|^2 + |a_2|^2 = 1$. See ref. [15] for further details on rotation properties for this system. Observe that the experiment is designed to study changes of the quantum state and not to measure the $z$-component of the spin-system (electron or anything in a state $S=1/2$). In the present approach, there is no particle model implied, quantum amplitudes are the fundamental elements. The amplitudes and base states belong to Hilbert space; the
Localization in real space is made with the help of the inertial frame in uniform motion. This defines a beam in our language.

Taking the y-axis as the beam’s propagation direction in the laboratory frame the origin is taken at the oven aperture. The quantum state including k-space elements of a beam along the y-direction can be written as a product, spin and space stationary states along z- and x-directions and a planar wave along the y-direction:

\[ <rl a_1 a_2, k_z, k_x, k_y> = F_0(k_r) (a_1 a_2) |+> |-> \]  \hfill (15)

Here,

\[ F_0(k_r) = (\exp(i k_z r) + \exp(-i k_z r)) (1/\sqrt{2}) (a_1 a_2) \]  \hfill (16)

Implicit in the right-hand side of eq.(15) is the linear superposition in the canonical spin basis \[ |+> |-> \]. This quantum state (i.e. the amplitudes) can be changed by the interaction with a Stern-Gerlach (SG) apparatus located, for instance along the z-axis; SG-z in Fig.1. To perform

the analysis of the interactions, consider the spin eigenstate \( |1 0 \rangle \). The state functions along the x- and y-axis are not perturbed by the interaction along the z-axis. The SG-z can produce a transition of the z-space part of Hilbert space with the following result:

\[ (\exp(i k_z r) + \exp(-i k_z r)) (1/\sqrt{2}) (1 0) \rightarrow + (\exp(i k_z r) - \exp(-i k_z r)) (1/\sqrt{2}) (1 0) \]  \hfill (17a)

And, analogously for the spin eigenstate \( |0 1 \rangle \), one gets

\[ (\exp(i k_z r) + \exp(-i k_z r)) (1/\sqrt{2}) (0 1) \rightarrow -(\exp(i k_z r) - \exp(-i k_z r)) (1/\sqrt{2}) (0 1) \]  \hfill (17b)

This reflects a transition between two transverse quantum states induced by SG-z on the physical state; the excited state that differs in one node from the ground state. The wave function after interaction is the sum of the unperturbed and perturbed parts. One gets either eqs. (18a) or (18b):
This result reflects, in real space, the directionality assigned by the interaction to the resultant quantum state. In Hilbert space, we have to reconstruct the state in the basis of spin functions. Equations (18a) and (18b) are the components in the basis $| + > | - >$. The common factor $(\exp(i k_x r) + \exp(-i k_x r)) \exp(i k_y r)$ shows that the quantum amplitude is “moving” along the $y$-direction only.

Let us consider now a general spin state, $(a_1 a_2) | + > | - >$. In Hilbert space one always has simultaneously both components. In real space, a screen can be put in order to get a detectable signal.

Here rises a puzzling situation if one interprets the wave function with a particle model. Assume that a signal is detected along the direction $\exp(-i k_z r)$, i.e. in the negative direction of the $z$-axis or $\exp(-i k_z r) (0 \ a_2)$. In this case, one takes for granted that a particle with spin $\beta$ has collided with the screen. Hilbert space representation tells us that both amplitudes have impinged on the screen; the one for positive $z$-axis direction is $\exp(i k_z r) (a_1 0)$. The particle model indicates that a transition from the state $|1> \approx \exp(i k_x r) \{ \exp(i k_x r) + \exp(-i k_x r) \} (\exp(-i k_z r) a_1 \ \exp(-i k_z r) a_2) |+ > \ | - >$ $(19)$ and

$$|2> = \exp(i k_y r) \{ \exp(i k_x r) + \exp(-i k_x r) \} (0 \ \exp(-i k_z r) a_2) |+ > \ | - >$$ $(20)$

But, now the coefficient in eq.(20) must be $a_2=1$ if the state $|2> \ \text{is normalized}$. In this “particle” model, the initial quantum state information, i.e. $(\exp(+i k_z r) a_1 \ \exp(-i k_z r) a_2)$ would be lost. In our view, this transition is more of a wishful thinking than an actual process.
The result gathered in eq.(19) is able to describe, accurately, the statistical results because the information on the spin state remains at disposal. If the experimentalist has prepared the initial quantum state as \((1 \ 0)\), then no measurement made along the negative \(z\)-direction would produce a signal; the reason is simple: the amplitude there will remain zero. While a measurement along the positive \(z\)-axis would produce a certain result because the amplitude is one. Observe that if the experimentalist prepares a linear superposition, \((1/\sqrt{2} \ 1/\sqrt{2})\), half of the measurement scores would appear upwards and the other half downwards; this result is applicable to an ensemble of systems. If we consider individual events, quantum mechanics does not allow predicting with exactness the outcomes of such events; it only says that it will (or may) happen.

Now we analyze a more complex situation than the one depicted in Figure 2. Consider the initial spin state as being \((1/\sqrt{2} \ 1/\sqrt{2})\). Let us apply a SG-\(z\) and in addition a SG-x on the linear superposition. After some algebra, the quantum state in the canonical basis \([|+\> \ |-\>]\) can be cast into four components:

\[
<r|\Phi> = \{(1 \ 1) \ 1/\sqrt{2} \ \exp(i \ k_z \cdot r) \ \exp(i \ k_x \cdot r) \ \exp(i \ k_y \cdot r) + \\
(1 \ -1) \ 1/\sqrt{2} \ \exp(-i \ k_z \cdot r) \ \exp(-i \ k_x \cdot r) \ \exp(-i k_y \cdot r) + \\
(-1 \ 1) \ 1/\sqrt{2} \ \exp(-i \ k_z \cdot r) \ \exp(i \ k_x \cdot r) \ \exp(i k_y \cdot r) + \\
(-1 \ -1) \ 1/\sqrt{2} \ \exp(-i \ k_z \cdot r) \ \exp(-i \ k_x \cdot r) \ \exp(-i k_y \cdot r)\} \ [|+\> \ |-\>] \quad (21)
\]

One obtains four amplitudes with different combinations of \(k\)-vectors. The system as a whole keeps modulated by \(\exp(i k_y \cdot r)\) so that it “moves” along the positive \(y\)-direction. Let us read the quantum state \(<r|\Phi>\) with local measuring apparatuses. This aspect of the problem is discussed below in more detail.
3.2. Reading recordings

The quantum state $<\mathbf{r}|\Phi>$ given by Eq.(21), or any recasting thereof, is all what there is in Hilbert space. The wave function is defined over the whole configuration space. There are no “beams” at sight in this space. This can be seen by recasting Eq.(21) in terms of the eigenstates $(1 \ 0)$ and $(0 \ 1)$. One gets eq.(22):

$$<\mathbf{r}|\Phi> = \{ (1/2\sqrt{2}) (\exp(i \mathbf{k} \cdot \mathbf{r})+\exp(-i \mathbf{k} \cdot \mathbf{r})) (\exp(i \mathbf{k} \cdot \mathbf{r})-\exp(-i \mathbf{k} \cdot \mathbf{r})) (1 \ 0) \exp(i \mathbf{k}_y \cdot \mathbf{r}) + (1/2\sqrt{2})(\exp(i \mathbf{k} \cdot \mathbf{r})-\exp(-i \mathbf{k} \cdot \mathbf{r})) (\exp(i \mathbf{k} \cdot \mathbf{r})+\exp(-i \mathbf{k} \cdot \mathbf{r})) (0 \ 1) \exp(i \mathbf{k}_y \cdot \mathbf{r}) \} [\mathbf{1}\mathbf{>} \mathbf{-}\mathbf{1}\mathbf{>}]$$

(22)

The recording of eq.(22) is not a problem because a reading device must be a recording device in the first place. Therefore, the Hilbert space has to be expanded to allow for a quantum mechanical definition of detection apparatuses.

The dilemma arises because the reading is to be carried out with a local device and a particle ideology is usually implicit to locality. For instance, one may want to use local spin flip state detection with a SG instrument. This is a problem demanding special treatment because eq.(22) is non local: the amplitudes to the states $(1 \ 0)$ and $(0 \ 1)$ indicate that a “spin-flip” would engage the global transition, namely, all four “beams” (Cf. eq.(21)) would be involved in the change of spin state. From this perspective, there is no local change of “spin” as if it were transported by a “particle”. These latter concepts belong to the realm of classical space-time physics.

To introduce the concept of reading a recording, boundary conditions must be defined for the reading device in real space-time. Moreover, a mechanism defining local response must be given. The nature of the new Hilbert space is determined by the nature of the instrument selected. For the example chosen of two SG apparatuses, the result over an ensemble is known: four spots will form. Note that while the system wave function is global, the detectors registering the four “beams” must be local.
Here pops up the problem because of the use of a yes-no response to define reading (eventually observing) a wave function imprint (registering). The analysis of this type of interaction requires the introduction of an appropriate basis in Hilbert space for the detectors. The general equations are certainly valid but a local measuring device should incorporate a yes-no mechanism as a necessary condition to be “seen” in real space. Now, to accomplish this goal, let the quantum basis state $|1\rangle$ be that for which there is a quantum of the measurable system at a given point, and $|0\rangle$ there is no quantum of the measurable system there (the quantum stands for whatever is the case). A quantum state of the detector (registering device) is then represented as the linear superposition: $(d_1, d_2) [|1\rangle \, |0\rangle]$. Standard normalization condition holds: $|d_1|^2 + |d_2|^2 = 1$. Therefore, the quantum state represented by the vector $(1 \ 0)$ means that there is a quantum of the measurable system at the location of the measuring device. The row vector $(0 \ 1)$ represents the situation where there is none apparent change there at the place where the detector is. Then, if after interaction the apparatus senses a change towards the state $(1 \ 0)$, this quantum change must be susceptible of amplification and, eventually, transformed into a “click”; here, we are well beyond linear quantum mechanics realm. This part of the process introduces irreversibility because a "click" reversion process is not in a one-to-one relationship with a particular imprint. Now, the measured quantum system must undergo a concomitant change (see below) to pay for the transition (not for amplifying the signal).

This is an extreme example used in fixing ideas. But one point is clear in this example. It is the experimenter that can introduce the locality and the irreversibility on the local device. One can suspect that after measurements with local devices, the interactions introduce locality elements in the measured wave function after interaction changing it into a new quantum state. A Hilbert space representation adapted to measurements on to the quantum state represented by eq.(21) is constructed now.

Let us consider one example. Four local devices are positioned along the directions $\mathbf{k}_M$: $(k_x, k_y, k_z)$, $(-k_x, k_y, k_z)$, $(k_x, -k_y, -k_z)$, $(-k_x, -k_y, -k_z)$, indicated by the k-vectors of the wave function (21) located on the same plane perpendicular to the y-axis (Cf. Fig. 2). The initial
The state of the whole measuring device may be represented by the linear superposition 
\[ |\Psi\rangle = |0\rangle_1 |0\rangle_2 |0\rangle_3 |0\rangle_4 |0\rangle_5 M \]
\[ |1\rangle_1 |1\rangle_2 |1\rangle_3 |1\rangle_4 |1\rangle_5 |0\rangle_6 |0\rangle_7 |0\rangle_8 |0\rangle_9 |0\rangle_{10} M . \]
The sub index stand for the local device located at \( xz, -xz, -x-z, x-z \) on the plane perpendicular to \( y \) axis, respectively. Each base vector is multiplied by \( \exp(-i k_{M_{h}} \cdot r) \), \( h=1,\ldots,4 \). For instance, \( |1\rangle_1 = \exp(-i k_{M_{1}} \cdot r) |1\rangle \), with \( k_{M_{1}} = (k_{x},k_{y},k_{z}) \). The simplest case would be to have read a signal in the detector 1 and none over the remaining detectors. The wave function of the composed system is the product of eq.(22) taken with \( \exp(-i k_{M_{1}} \cdot r) \) \( <r|l\rangle \). Using the representation given by eq.(21), the amplitude reads as:

\[ <r|\Phi\rangle \exp(-i k_{M_{1}} \cdot r) <r|l\rangle = \frac{1}{\sqrt{2}} \left\{ (1 \ 1) + (1 \ -1) \exp(-i 2k_{x} \cdot r) + (-1 \ 1) \exp(-i 2k_{x} \cdot r) + (-1 \ -1) \exp(-2i k_{z} \cdot r) \exp(-2i k_{x} \cdot r) \right\} <r|l\rangle [|> + |-] \] (23)

Now, the boundary condition designating the detector in real space is incorporated. Integrating over the detector surface of macroscopic size leads to cancellation of all but the first term because the integrals over the exponential terms oscillate rapidly.

\[ (1 \ 1) \frac{1}{\sqrt{2}} <r|l\rangle [|> + |-] A_{1} \] (24)

This response is proportional to the area of the detector \( A_{1} \).

Now, a reading in intensity regime (“clicking” counting) at the detector is defined by taking the square modulus after simplifying \( <r|l\rangle \) and taking a unit surface, \( A_{1}=1 \). One can see that 1/8 of the intensity will come from the spin state \( (1 \ 0) \) and 1/8 for the spin state \( (0 \ 1) \), both adding up to 1/4. This is the expected statistical result. Therefore, when expressed as intensity, the brute response revealed by a simple “click” contains the propensity conveyed by the linear superposition (eq.(22) or the equivalent eq.(21)) locally projected. If one refers to an ensemble, the results in intensity regime obtained here coincide with the standard statistical representation.

There is an important caveat. In the present theory, eigenvalues as such are not the observable in a direct fashion. This is clearly seen in the structure of eqs. (3,4) etc. The
amplitude to be correlated to the standard theory must be the one where all "external" factors are removed, namely eq.(25):

\[
\left( \int dx \, dz \, \langle r|\Phi\rangle \exp(-i k_{M_1}.r) \langle r|1\rangle / \langle r|1\rangle \right) A_1 = (1 \quad 1) \frac{1}{\sqrt{2}} [|+\rangle \quad |-\rangle]
\]

The integration in the left-hand side is carried out only over the plane perpendicular to the y-axis. This is integration in "real space" induced by the measuring apparatus. The RII gives now exactly the same result as the statistical approach. How does one represent the case where no “click” was detected at M\(_1\) and no other detector is present elsewhere? The result can be worked out by using the amplitudes and properties of the detector. We have now the amplitude to the \(\langle r|0\rangle\) wave function:

\[
\langle r|\Phi; M_1\rangle = (1 \quad -1) 1/\sqrt{3} \sqrt{2} \exp(i k_x . r) \exp(-i k_y . r) +
\]

\[
(1 \quad -1) 1/\sqrt{3} \sqrt{2} \exp(-i k_x . r) \exp(-i k_y . r) +
\]

\[
(1 \quad -1) 1/\sqrt{3} \sqrt{2} \exp(-i k_x . r) \exp(i k_y . r) \langle r|0\rangle \quad [|+\rangle \quad |-\rangle]
\]

The function \(\langle r|0\rangle\) is localized over a small volume of detector M\(_1\) and can be taken to be independent of \(r\) when integration over the area of the detector is performed (this is the new boundary condition). This factors out in both sides of eq.(26) and cancels out. The term \((1 \quad 1)\)

\[
1/\sqrt{2} \langle r|0\rangle \quad [|+\rangle \quad |-\rangle]
\]

is hence a constant and is taken away. The modified amplitude will be now:

\[
\langle r|\Phi; M_1\rangle = (1 \quad -1) 1/\sqrt{3} \sqrt{2} \exp(i k_x . r) \exp(-i k_y . r) +
\]

\[
(1 \quad -1) 1/\sqrt{3} \sqrt{2} \exp(-i k_x . r) \exp(i k_y . r) +
\]

\[
(1 \quad -1) 1/\sqrt{3} \sqrt{2} \exp(-i k_x . r) \exp(-i k_y . r) \exp(-i(k_y (r - r_{M_1})) \quad [|+\rangle \quad |-\rangle]\]

The result of the idle reading interaction manifests in that the spin data and the phases have been altered when compared to eq.(22). The origin of the propagating plane wave along the y-axis has now been shifted to the position \(r_{M_1}\) of the detector plane and the linear superposition
is normalized to one again. The important result is that even the idle interaction can change
the wave function of the measured system.

A preparation experiment can also be described in the present context. Consider the
case where we put 3-detectors, M$_2$, M$_3$ and M$_4$. Selecting the cases where these three detectors
do not "click", the global system (Cf. eq(22)) changes the coherence pattern into the one
represented by eq.(28):

$$<x|\Psi> \exp(i k \cdot (r-r_{M1})) \exp(-i (k/\sqrt{2})(r-r_{M1}))(1/\sqrt{2}) [\dagger\rightarrow]$$  (28)

This new quantum state can be submitted to SG experiments. Note the difference between
eq.(25) and (28). For eq.(25) the amplitude corresponds to "clicking response" situation, the
numerical coefficients are then related to those of eq.(21), while in (28) a new quantum
amplitude obtains; here, no particle is implied as the state is (1/\sqrt{2}  1/\sqrt{2}).

The analyses presented above show that local interactions might serve multiple
purposes. For instance, the reading of quantum recordings and change of coherence patterns.
Preparation of a quantum system in a given quantum state (Cf. Eq.(28)) can also be achieved
with local measuring apparatuses. Mirror devices give another example, not discussed here.
They change the longitudinal part of the k-state of systems leading then to possible local
changes of coherence patterns. As seen in the example above, the interaction may lead to local
effects susceptible to be measured or the amplitude may be used to enter again in a quantum
interaction (interference experiments).

There are many ways to detect the interaction between measured and measuring
quantum amplitudes. However, the amplification can be easily understood as a process
occurring in the [\dagger\rightarrow] Hilbert space with effective energy exchange. The counting leads to
populations. Populations are used to define probability measures. The standard theory of
measurement corresponds to the transformation of a pure state into a mixture
$$\rho = \sum |C_n|^2 P_n .$$
Taking tr\rho =1 the intensity measurement can be expressed in the language of Kolmogorov’s
probability scheme. In our approach this situation will be true if and only if an intensity reading is implied.

Nevertheless, as discussed above, reading-in-amplitude is also allowed. The RIA permits understanding interference behavior that is the blue print of quantum physical processes [12]. The conclusion is that irreversibility does not make an integral part of the measurement process. It only shows up in special cases.

5. Discussion

We have presented a simple physical model to describe measurements in a quantum setting. One starts with a single initial quantum state, namely a set \{a_j b_k\} and after the interaction has taken place a single final quantum state \{a_j' b_k'\} is produced. Thereafter, a reading process was defined. Two classes were identified: reading-in-intensity and reading-in-amplitude. We take the existence of these classes of readings as a fundamental hypothesis.

A blueprint of classical macroscopic nature will then be a local intensity-measuring device. However, this will only be an aspect of macroscopic systems because they can also show, in a particular spectral region, quantum mechanical response: i.e. reading-in-amplitudes capabilities. A pure quantum system, however, would only have the reading-in-amplitude property.

The initial state \{a_j b_k\} can also be representing a reacting n-electrons and m-nuclei system coupled to a thermal bath at a given absolute temperature T. The quantum molecular base states is the infinite set of electronuclear wave functions constructed on the basis of generalized electronic diabatic (GED) functions. For more details the reader can examine references [7;20;4;5]. The base states are labeled with two quantum numbers: electronic and a nuclear one; this latter gather the vibration, rotation and translation degrees of freedom; but, for simplicity they are designated as \{|s_n>\} with n=0,1,2,... The electronic state defines a chemical species [4]; among them, all possible sets of ionized as well clusters are to be
included; charge and mass conservation is required. A quantum state of a reacting system (take a unimolecular ground state case to fix ideas) is given by:

\[ |\psi\rangle = (a_1, \ldots, a_n, \ldots) [|s_1\rangle, \ldots, |s_n\rangle, \ldots] = a_\mathbf{s} = \sum_n a_n |s_n\rangle \]  \hspace{1cm} (29)

The system D is taken to be an appropriate quantized electromagnetic (EM) field, a laser pulse or blackbody radiation. All frequencies required for a resonant interaction can be manipulated in the laboratory. If we eliminate from this model the spontaneous emission and retain only the stimulated emission, the entanglement between both systems is formally avoided. Let us prepare the system in its ground electronic state: \((1 \ 0 \ 0 \ 0 \ldots 0 \ldots)\). By ordering the electronic states according to the energy of their stationary geometry the chemical species are ranged according to increasing electronic energy. Assume the state \(i=5\) is characterized by its own set of topologic indexes \[4\]; the quantum state \((0 \ 0 \ 0 \ 0 \ 1 \ 0 \ldots 0\ldots)\) represents a “pure” species; a product of a chemical change. In the standard quantum chemical approach, the base state represents a substance in real space. In the present view, all possible chemical species including vibration, rotation and translation spectra are given once and for all; the base states belong to Hilbert space. The only thing that would change is the amplitude as interactions with external sources (sinks) of energy are made available. Let us prepare the thermal bath so that we know its quantum state: \(\{b_k(t_0)\}\). The initial state of the system is then \(\{a_j b_k\} = \{a_j(t_0) b_k(t_0)\}\). Let them interact. Bring the reactant system away the bath and determine the new set of amplitudes, \(\{a'_i, b'_k\}\)=\(\{a_j(t_f) b_k(t_f)\}\). If the interaction time was sufficiently long, the set \(\{a'_i\}\) represents the amplitudes of a system in thermal and chemical equilibrium provided there is no kinetic bottlenecks. And that’s it. A chemist, however, may be interested in the state \((0 \ 0 \ 0 \ 0 \ 1 \ 0 \ldots 0\ldots)\), that is, the “pure” thing. This person, not theoretically representable, would know how to precipitate the system corresponding to \(i=5\) thereby introducing unpredictable (for us) events. Before such intervention, chemical evolution can be seen as a full-fledged quantum mechanical time evolution \[7;4\]. Observe that we can read the chemistry from \(\{b_k(t_f)\}\) if we care about the bath by measuring its spectra. This is the normal procedure to study interstellar chemistry.
Experimental conditions can be created that prevent substantial influence of spontaneous emission on the results. The measurement theory described here can be adapted to this new situation. To illustrate this point consider an S-system having three well isolated electronic states with energies $E_1 < E_3 < E_2$. The resonance frequencies being $\nu_{12} = (E_2 - E_1)$ and $\nu_{32} = (E_2 - E_3)$; $\hbar/2\pi = 1$. The transition moment between states 1 and 3 is taken to be zero and $\nu_{12} \gg \nu_{32}$. Now, let us perform an experiment in three stages. First, send a laser pulse around frequency $\nu_{12}$ matching the resonance with the system S. A photon is absorbed and subsequently emitted via stimulated emission mechanism. The signal is then going in the same direction as the laser pulse. Second experiment, with the laser at $\nu_{12}$ on, one switches on a second laser resonant to the transition $\nu_{32}$. This laser stimulates the emission from level 2 to level 3. If the second laser is now switched off, energy is accumulated in level 3. The system S has now read both fields and got an imprint in it. Third experiment, the imprinted system is now “re-excited” with the small $\nu_{32}$ frequency. The level 2 now can re-emit in the direction of the first laser light pulse as long as coherence has not been lost. The key issue is that all phase information was stored in the S-system as if it were a quantum-measuring device. As a matter of fact, such experiments have been done on Bose-Einstein condensate [21]. A more correct description of these phenomena would involve coherent evolution of quantum amplitudes rather than a population-like description.

The present approach demands an interpretation of the quantum mechanical symbols that differ from the standard one [22;17]. To which extent the present approach is more advantageous than the standard one is not an issue for the present paper. Thorough experimental tests will have the last word, as there are a number of predictions [12] differing from the standard theory.
References


