# Reality and Causality in the Microscopic World: A Discussion from Quantum Transport Theories

Chapter on "Physics and the Nature of Reality: Essays in Memory of Detlef Dürr".

#### Abstract

Paraphrasing Feynmann, perhaps, the main reason why the so-called Copenhagen (or orthodox) quantum theory is so popular among the physicists and engineers is because "I can safely say that nobody understands [it]". Many physicists and engineers take profit of the mathematical machinery of the Copenhagen theory without paying attention to its ontology, which implies that a quantum object has no microscopic properties (unless a property is measured, or the quantum object is an eigenstate of some property). Such an orthodox view of a microscopic world, empty of properties, is specially unsuitable to understand and to develop approaches to predict modern nanoelectronics, as we discuss along this chapter. As an alternative, physicists dealing with the foundations of quantum transport and open systems have developed different approaches in terms of some type of causal motion of electrons. When dealing with nanodevices, the Copenhagen ontology affirms that electrons are nowhere since their positions are undefined until measured, while causal motion approaches say that electrons can be perfectly understood as particles traversing a device with well-defined positions, independently of the measurement. This last view certainly holds true for treatments based on the Bohmian theory. Even for quantum phenomena of light, such as spontaneous emission or photon partition noise, the Bohmian theory allows an explanation from well-defined electromagnetic fields interacting with electrons, which is contrary to the standard Copenhagen approach. The above examples, developed in this chapter, emphasize that the main merit of the Bohmian theory is eliminating the observer/measurement as the "creator" of the microscopic reality, showing that a well-defined description at all times, of the microscopic properties of a quantum system, is available (where particles are particles and fields are fields at all times). Such a microscopic description does not only provide conceptual advantages, but also important numerical ones when electron devices are understood, in general, as non-Markovian open quantum systems.

In front of the incapacity of the standard quantum theory (so called Orthodox interpretation), to answer "when", "for how long" or whether there "are" electrons crossing the transistors of our phones at all, any physicist or engineer that needs to consider that this is indeed the case for the practical development of cutting edge devices, resorts to alternative explanations of quantum phenomena in terms of electrons that actually do cross their transistors [1]. The well known Bohmian explanation is one such alternative to the Orthodox interpretation [2, 3, 4, 5].

As an example of how impractical the limitations of the Orthodox view can arrive to be: in its terms, it is still obscure something as fundamental for modern electronics as is the current measurement for nano-devices operating at high frequencies [6]. Not for interpretative issues alone, but mainly due to **practical** issues like the search of an operator for the multi-electron current observable, or the requirement to treat a high frequency measuring apparatus as a non-Markovian environment. As we will discuss along the chapter, satisfying and practically useful explanations for these, apparently seem to demand the use of modal theories like Bohmian mechanics.

The essential tools for reaching these conclusions are the concepts of conditional wave-function (CWF) and effective wave-function (EWF) introduced by  $D\ddot{u}rr$  et al. in Ref. [7], together with the understanding of the measurement dilemma they enlighten. Thus, we will first detail all of these concepts, so we can then naturally conclude solutions for the aforementioned practical limitations.

## The Conditional and Effective Wavefunctions

Given a quantum system of N degrees of freedom described by the real coordinate vector  $\vec{X} = (x_1, ..., x_N) \in \Omega_t \subseteq \mathbb{R}^N$ , we can describe its evolution in continuous time  $t \in \mathbb{R}$ , with the use of a complex wavefunction  $\Psi(\vec{X}, t) = \rho^{1/2}(\vec{X}, t)e^{iS(\vec{X}, t)/\hbar}$  (encoding the two real fields S and  $\rho$ ), and an associated Bohmian trajectory  $\vec{X}^{\vec{\xi}}(t) \equiv \vec{X}(\vec{\xi}, t)$  the initial condition of which is given by the label space vector  $\vec{\xi} \in \Omega_0 \subseteq \mathbb{R}^N$  such that  $\vec{X}^{\vec{\xi}}(t=0) = \vec{\xi}$ . This trajectory is guided by the wavefunction through the "guidance law", while the wavefunction itself is guided by the Schrödinger Equation [2, 3, 4, 5]. Respectively:

$$\frac{\mathrm{d}x_k^{\xi}(t)}{\mathrm{d}t} = v_k(\vec{X}, t) \Big|_{\vec{X} = \vec{X}^{\xi}(t)} := \frac{1}{m_k} \frac{\partial S(\vec{x}, t)}{\partial x_k} \Big|_{\vec{X} = \vec{X}^{\xi}(t)}$$
(1)

$$i\hbar \frac{\partial \Psi(\vec{X}, t)}{\partial t} = \left[ \sum_{k=1}^{N} \frac{\hbar^2}{2m_k} \frac{\partial^2}{\partial x_k^2} + U(\vec{X}) \right] \Psi(\vec{X}, t)$$
 (2)

where  $m_k$  is the mass associated with the k-th degree of freedom,  $v_k$  is the velocity field piloting the k-th degree of the Bohmian trajectories and U denotes the classical potential describing the interaction between the degrees of freedom (since we consider an isolated system we assume no time dependence, but we could describe in general a closed system by allowing it to vary in time).

The most general isolated system we could consider is the whole Universe, where  $\vec{X}$  would reflect its degrees of freedom or space of **configurations**. We can partition it in a subsystem of interest S, of say, n < N degrees of freedom, labeled by  $\vec{x} = (x_1, ..., x_n)$ , and its environment E, of configuration coordinates  $\vec{y} = (x_{n+1}, ..., x_N)$ , such that  $\vec{X} = (\vec{x}, \vec{y})$ . We could associate one wavefunction to S and one to E, both labeled by the initial global trajectory configuration  $\vec{\xi}$ , respectively as  $\psi^{\xi}(\vec{x}, t) := \Psi(\vec{x}, \vec{y}^{\xi}(t), t)$  and  $\phi^{\xi}(\vec{y}, t) := \Psi(\vec{x}^{\xi}(t), \vec{y}, t)$ . These are particular cases of the so called **conditional wavefunctions** (CWF-s). In general, a CWF is just evaluating some of the degrees of freedom of a wavefunction along a (Bohmian) trajectory for them, while leaving the rest un-evaluated [7, 5].

As proved in [8], the full Schrödinger Equation (2), ruling the dynamics of the whole system, can be re-written exactly into two coupled dynamical sets of equations ruling the motion of the two presented CWF-s. For the S (for the E they will be the same but changing the indexes and the CWF):

$$i\hbar \frac{\partial \psi^{\xi}(\vec{x},t)}{\partial t} = \left[ \sum_{k=1}^{n} \frac{\hbar^{2}}{2m_{k}} \frac{\partial^{2}}{\partial x_{k}^{2}} + U(\vec{x}, \vec{y}^{\xi}(t)) + G(\vec{x}, \vec{y}^{\xi}(t), t) + i J(\vec{x}, \vec{y}^{\xi}(t), t) \right] \psi^{\xi}(\vec{x}, t)$$
(3)

with G and J the real and complex parts of the so called quantum correlation potential:

$$G(\vec{x}, \vec{y}^{\xi}(t), t) = \sum_{j=n+1}^{N} \left[ -\frac{1}{2} m_j \left( v_j(\vec{x}, \vec{y}^{\xi}(t), t) \right)^2 - \frac{\hbar^2}{2 m_j \rho^{1/2}(\vec{x}, \vec{y}^{\xi}(t), t)} \left( \frac{\partial^2 \rho^{1/2}(\vec{x}, \vec{y}, t)}{\partial x_k^2} \right) \Big|_{\vec{y} = \vec{y}^{\xi}(t)} \right]$$
(4)

$$J(\vec{x}, \vec{y}^{\xi}(t), t) = -\frac{\hbar}{2} \sum_{j=n+1}^{N} \frac{\partial}{\partial x_j} v_j(\vec{x}, \vec{y}, t) \Big|_{\vec{y}^{\xi}(t)}$$

$$(5)$$

where we recognize as G the difference between the quantum potential [5, 4] and the kinetic energies of the trajectory of the E (the Lagrangian of the E) and as J, the spatial variation of the Bohmian velocity of the E in its coordinates. All these are terms that involve a derivative of the phase S or the magnitude  $\rho$  of the full wavefunction  $\Psi$  in the E coordinates  $\vec{y}$  centered at the trajectory position  $\vec{y}^{\xi}(t)$ . This means that in order to compute them, we would not have enough with the two CWF-s veloce to but not exactly in  $\vec{y}^{\xi}(t)$ . This is an explicit manifestation of the so called quantum wholeness [5], by which the dynamics of a single Bohmian trajectory depends on the dynamics of the rest of possible trajectories. Thus, we see that while U introduces all the classical correlation between the S and the E, the responsible ones for their quantum interaction (and the interaction with the rest of possible Bohmian trajectories) are G and G.

Now, if the imaginary potential J vanished for the S, we see that the CWF  $\psi^{\xi}(\vec{x},t)$  would behave as if it was a closed quantum system wavefunction, ruled by the unitary evolution of a Schrödinger Equation (2), where the potential energy would now be a time dependent one:  $V(\vec{x},t) = U(\vec{x},\vec{y}^{\xi}(t)) + G(\vec{x},\vec{y}^{\xi}(t),t)$ . Yet, computationally, we would still require a quantum description for the E in order to evaluate G. Thus, only if we also made G negligible, would the S behave exactly as an independent closed quantum system, only interacting with the E classically (through U). Whenever this is the case, we can say that the CWF of the S is the **effective wavefunction** (EWF) of the S.

The question is then: when are J and G (the quantum influences of the E on the S) negligible? When the full wavefunction's variation along the axes of the E,  $\vec{y}$ , in the neighborhood of its trajectory  $\vec{y}^{\xi}(t)$ , is negligible:  $\frac{\partial \Psi(\vec{x}, \vec{y}, t)}{\partial x_j}|_{\vec{y}=\vec{y}^{\xi}(t)} \simeq 0 \quad \forall j \in \{n+1, ..., N\}$ , both G and J will vanish, as they involve derivatives of the magnitude  $\rho^{1/2}$  and the phase S of the wavefunction  $\Psi$  in the axes of the E,  $\vec{y}$ , around  $\vec{y}^{\xi}(t)$ . For example, this is the case when the CWF-s of the S,  $\psi^{\xi}(\vec{x}, t)$ , are significantly different only if macroscopically distant CWF-s are considered (along  $\vec{y}$ ), or when equal CWF-s of the S are piled in macroscopically distant and disjoint supports in configuration space, as we will see.

#### Measurement understood as unitary evolution using Bohmian CWFs and EWFs

Given the initially closed quantum system S and its EWF  $\psi(\vec{x},t)$ , to take a projective measurement of its property G, as suggested by von Neumann [9] and explained in terms of Bohmian mechanics in Refs. [4, 5, 3], we can consider the position of the dial of a measuring apparatus M, or the generalized coordinate of such an indicator, which is what is observed by the experimenter. Lets call it  $z \equiv x_{n+1}$  (it is part of the environment of the S). We prepare the EWF of this dial to be a fiducial state that will make sure its Bohmian position at the first time of the measurement t=0, that is  $z^{\xi}(t=0)$ , is reliably around the macroscopic rest position of the dial z=0, with a high precision and accuracy. For example  $\varphi(z,t=0)=ce^{-z^2/4\sigma^2}$ , or in ket notation  $|\varphi(t=0)\rangle_M=\int_{\mathbb{R}}\varphi(z,t=0)|z\rangle\,dz$ , with  $c=1/((2\sigma\pi)^{1/4})$  a normalization constant and  $\sigma$  not macroscopically distinguishable. We now let the EWF of the S, which in ket notation is  $|\psi(0)\rangle_S=\int_{\mathbb{R}^N}\psi(\vec{x},0)\,|\vec{x}\rangle\,dx$ , interact with the measurement dial through the

<sup>&</sup>lt;sup>1</sup>Note that while information about multiple stacked CWF-s for the S around  $\vec{y}^{\xi}(t)$  is required to compute G and J, the guidance for the trajectory of the S,  $\vec{x}^{\xi}(t)$ , is given entirely by the CWF of the S at  $\vec{y}^{\xi}(t)$ :  $\psi^{\xi}(\vec{x},t) = r^{\xi}(\vec{x},t)e^{is^{\xi}(\vec{x},t)/\hbar}$ , as  $\frac{\mathrm{d}}{\mathrm{d}t}x_k(t) = \frac{1}{m_k}\frac{\partial s^{\xi}(\vec{x},t)}{\partial x_k}\Big|_{\vec{x}=\vec{x}^{\xi}(t)}$  for  $k \in \{1,...,n\}$ . That is, if it was not for G and J, the CWF would behave itself as a Schrödinger equation wavefunction.

von Neumann Hamiltonian  $\hat{H}_{MS} = \mu(t)\hat{p}_M \otimes \hat{G}_S$ , where  $\hat{p}_M$  is the momentum operator of the dial z and  $\hat{G}_S$  is the operator related with the property G of the S we wish to measure.  $\mu(t)$  is the interaction strength which has support only in  $t \in (0,T)$  (the interaction time), such that  $\mu := \int_0^T \mu(t) dt$ .

If the observable G has countable spectrum, such that  $\hat{G}_S = \sum_k g_k |g_k\rangle_S \langle g_k|_S$  with  $\{|g_k\rangle_S\}_k$  an orthonormal basis of S and  $|\psi(0)\rangle_S = \sum_k \alpha_k(0) |g_k\rangle_S$ : at the last interaction time t = T, the unitary Schrödinger evolution  $\hat{U}_0^T = e^{-i\mu T \hat{H}_{MS}/\hbar}$  will leave the composed state  $|\Phi(0)\rangle_{MS} = |\varphi(0)\rangle_M \otimes |\psi(0)\rangle_S$  as:

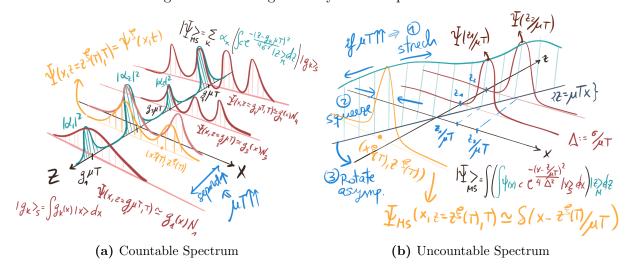
 $|\Phi(T)\rangle_{MS} = \sum_{k} \alpha_k(0) \left( \int ce^{-\frac{(z-g_k\mu T)^2}{4\sigma^2}} |z\rangle_M dz \right) |g_k\rangle_S$  (6)

This means, as graphically shown in Figure 1, that if the interaction strength  $\mu$  or time T are big enough, or  $\sigma$  is small enough, the probability density for the Bohmian position of the dial z, will be exclusively concentrated in several roughly disjoint Gaussians of weights  $|\alpha_k(0)|^2$ , each centered in a different  $g_k\mu T$  position in z, around which, the (normalized) CWF for the S is roughly constantly  $|g_k\rangle$ . The different Gaussians enveloping each eigenstate for S are macroscopically disjoint in z, since other-wise the dial would not be able to let us know the result of the measurement. Therefore, the CWF obtained by evaluating the observed Bohmian trajectory of z at t=T is an EWF, which turns out to be the eigenstate  $|g_k\rangle_S$  linked with the eigenvalue  $g_k$  indicated by z. Finally, the interaction between M and S is set off for times t > T, meaning the composite Hamiltonian  $\hat{H}_{MS}(\vec{x}, z, t)$  becomes  $\hat{H}_S(\vec{x}, t) + \hat{H}_M(z, t)$  for t > T, and as such, the evolution of the (normalized) CWF for the S (which is an EWF) can be made as if it was a closed quantum system fully independent of the M [5].

If the observable G had a continuous spectrum, such that  $\hat{G}_S = \int g |g\rangle_S \langle g|_S dg$  with  $\{|g\rangle_S\}_g$  an improper-state rigged Hilbert space orthonormal basis for the S, with  $|\psi(0)\rangle_S = \int \psi(g,0) |g\rangle dg$ , then the unitary coupling evolution will yield the following composed state at time t = T:

$$|\Phi(T)\rangle_{MS} = \int \left( \int \psi(g,0) c e^{-\frac{z}{\mu T})^2} |g\rangle_S dg \right) |z\rangle_M dz \quad \text{with} \quad \Delta := \frac{\sigma}{\mu T}$$
 (7)

where, as graphically shown in Figure 1, if  $\mu$  or T are big enough, or  $\sigma$  is small enough, the resulting wavefunction is stretched in z such that the variation is so slow in z, that if the interaction between the S and M is stopped for t > T, the S will be in an EWF equal to the CWF sliced by evaluating z in the observed Bohmian position  $z^{\xi}(T)$ . This EWF will be a very narrow Gaussian around  $g = z^{\xi}(T)/(\mu T)$  (tending towards a Dirac delta), and will be the EWF of the S with a probability density roughly equal to  $|\psi(z^{\xi}(T)/(\mu T), 0)|^2$  (the norm of the CWF). We know the state will need to be macroscopically stretched for our measuring dial to show significantly different positions.



**Figure 1:** Representation of the effective collapse of a 1D (n = 1) system, as explained in the text. In yellow the CWF of the system, which will be the EWF when normalized.  $N_k$  represents the norm of the CWF. In (a), a general countable spectrum observable  $\hat{G}$  is measured, in (b) a particular uncountable spectrum, the position operator  $\hat{x}$ , is measured.

In both cases, as seen from the S alone, it will have looked like the unitarily evolved state  $|\psi\rangle_S$  "collapsed" into one of the eigenstates of  $\hat{G}_S$ , with a probability equal to the pre-measurement state's projection magnitude squared  $|\alpha_k(0)|^2$  (or pdf  $|\psi(g,0)|^2$ ). This EWF will now continue to be unitarily and independently evolvable (for it will be an EWF with no interaction with M). The randomness of the measurement thus, arises due to the fact that we cannot know  $z^{\xi}(0)$  with an arbitrary precision, unless we made a projective measurement on it before the experiment. But such a measurement as seen, would require the coupling with another ancilla indicator and so on, until the chemicals in the perception of the observer, which is known as the von Neumann chain of observation [9].<sup>2</sup> The point is that a proper description of this chain (like the Bohmian one), allows us to decide where arbitrarily between the observer and the S we place the effective "collapse", which was a requirement placed by von Neumann himself [9, 10] over his axiomatization even if it is mainly ignored by the Orthodox<sup>3</sup>.

Now, either the assumption that for time t > T, M does not interact anymore with the S, or that the environment entanglement with the S is lost by some sort of thermalisation, mean that the information of the subsystem that was "leaked" to the environment (the so called "empty waves", which are the rest of CWF-s that are not sliced at  $z = z^{\xi}(T)$ ), do not interact back<sup>4</sup> with the EWF of the S. Any of these two assumptions thus imply that the environment effectively forgets the entanglement achieved with the S. This is an environment behavior we could call memory-less or Markovian.

Since the description of the E will only be useful for the measurement time interval (0,T), and we can then discard it (as we consider it for an ideal measurement to be Markovian), we can instead explain the projection of the state of the S to a subspace of its Hilbert space, with a set of effective"collapse" orthogonal projectors  $\{\hat{\Pi}_k\}_k$  without the need to explicitly formalize M [4]. We shall not forget however that this is just a short-cut in the modeling.

If we were now interested on the post-measurement description of the S, but irrespective of the measured result, we could independently unitarily evolve each of the different possible projected states (EWF-s), remembering which was the probability for each of them. Then if a second measurement is performed at a later point, we could simply treat another branching "collapse" on each of the independent states and weight them with the joint probability of the previous and the current measurements. For the sake of compactness, we could instead build a "matrix" operating on states where we set the orthogonal EWF-s as the ket-bra-s with their probabilities as coefficients. If we now apply a linear operator and its Hermitian conjugate at each side of the matrix (say, a unitary evolution), we will be applying the operator to each state-vector independently of the rest. Just as we wanted. Thus, we define an operator on state-vectors, to be used as a "possible state-probability pair" container:

$$\hat{\rho}_S(T) = \sum_k |\alpha_k(0)|^2 |g_k\rangle_S \langle g_k|_S \quad \text{or} \quad \hat{\rho}_S(T) = \int |\psi(g,0)|^2 |g\rangle_S \langle g|_S dg$$
 (8)

This is the so called **density matrix** of the S [9, 4, 3]. Note that for subsequent unconditional measurements, measurements in which we wish to keep track of all possible outcomes, the density matrix will get more and more mixed (the squared trace will diminish).<sup>5</sup> We say it is pure when we can represent it as a container describing a state with probability 1.

<sup>&</sup>lt;sup>2</sup>In reality, we cannot really couple the apparatus dial M directly to the S, nor we as observers with organic detectors are directly coupled to the dial M. Yet, we can couple the S to an order of magnitude bigger ancilla  $A_1$ , which will be coupled to a bigger ancilla  $A_2$ , and so on until M, and then until our perceptual observation, which due to the determinate Bohmian trajectory of its constituents, lets us know the result of the measurement. This discussion is in fact a restatement of the absolute uncertainty [7].

<sup>&</sup>lt;sup>3</sup>He did not believe in a physical collapse [10], instead he believed an explanation of the measurement should be possible setting an apparent collapse at an arbitrary point of the measurement von Neumann chain, which is what we allow with the Bohmian description.

<sup>&</sup>lt;sup>4</sup> They technically could if say, their macroscopic separation was made microscopic again.

<sup>&</sup>lt;sup>5</sup>Note that these are "diagonal" representations of the density matrix but we could equivalently express them in other bases, which means we can loose the microscopic deterministic detail of what is happening if the density matrix is all that is specified. Yet, for a probabilistic operational description of S (an epistemological description), this will suffice as we will see. Also keep in mind that if the Universe is to be taken as a pure state, a density matrix can always be seen as representing human uncertainty about a subsystem [11], letting our Bohmian view of the density matrices consistent.

### A Bohmian Narrative for General Quantum Operations

At this point, notice that the effective-"collape" due to a macroscopic separation in configuration space for different CWF-s, is not necessary to be part of a measurement by an observer. It could also happen as the effect of a more general environment coupling. For example, if part of the environment gets entangled with S and this environment is projectively measured, the S will also seem to suffer an effective-"collapse", but now into non-necessarily orthogonal nor linearly-independent states (nor a number of states limited by the dimensionality of the S Hilbert space).

This example is in fact what is called a **generalized measurement** [11, 4]. Given a decomposition of an initial state  $|\psi\rangle_S$  in a sum of not necessarily linearly-independent states of S and an independent fiducial state  $|\theta\rangle_A$  for an ancilla A, by using a suitable unitary  $\hat{U}_{AS}$ , we could couple each state of the decomposition of  $|\psi\rangle_S$  with a different state of an orthonormal basis  $\{|m\rangle_A\}_m$  of A:  $\hat{U}_{AS} |\theta\rangle_A \otimes |\psi\rangle_S = \sum_m |m\rangle_A \otimes |\psi_m\rangle_S$  where  $|\psi_m\rangle_S := \langle m|_A \otimes \hat{I}d_S (\hat{U}_{AS} |\theta\rangle_A \otimes |\psi\rangle_S)$  is an unnormalized S state called the **conditional state** of S for the m-th observation of the environment A. If we now perform an ideal projective measurement on A for the  $\{|m\rangle_A\}_A$  basis (coupling a dial M to A and branching A in EWF-s consisting of the measured eigenstates), ancilla-subsystem (unnormalized) EFW-s  $|m\rangle_A \otimes |\psi_m\rangle_S$  would be generated as a function of the Bohmian position of the dial. The m-th result would be observed with a probability equal to the norm squared of its conditional state  $N^2 := |\langle \psi_m | \psi_m \rangle|^2$ . If we then set-off the interaction between A and S for all future times, the S will have seemed to "collapse" into the EWF  $|\psi_m\rangle_S/N$  with probability  $N^2$ , since it will now evolve independently of A (Markovian).

As with the projective measurement of S, we can shortcut the formalization of the A and its measurement, by just considering the general measurement operators on the S (called POVM-s)  $\{\Omega_m := |m\rangle \otimes \hat{I}d\hat{U}_{AS}|\theta\rangle_A\otimes\}_m$ . The only requirement for them is:  $\sum_m \Omega_m^\dagger \Omega_m = \hat{I}d_S$ , so that the m-probabilities add-up to one, which is satisfied because  $\Omega_m |\psi\rangle_S = |\psi_m\rangle_S$  is the (unnormalized) conditional state, the squared norm of which is the probability to observe m [11, 4]. The reason why such an A and  $\hat{U}_{AS}$  exist for any set of linear operators  $\{\Omega_m\}_m$  satisfying the stated restriction, will be seen in a moment. Note that we could describe the post-measurement S unconditionally, using the density matrix idea just the same way as with projective measurements, defining  $\hat{\rho}_S = \sum_m |\psi_m\rangle_S \langle \psi_m|_S$  (or an integral). A second measurement on S would straightforwardly further mix the matrix.

The so called partial trace operation is tigthly related to this. Given a density matrix  $\hat{\rho}_{AS}$  for a composite  $A \otimes S$  and an arbitrary orthonormal base of the A,  $\{|m\rangle_A\}_m$ , the partial trace of  $\hat{\rho}_{AS}$  over A is defined as:  $tr_A[\hat{\rho}_{AS}] := \sum_k \langle m| \otimes \hat{I}_S(\hat{\rho}_{AS}) | m \rangle \otimes \hat{I}_S$  (or an integral if the "base" is made of uncountable improper states) [11, 4]. We call the result, the **reduced density matrix** of S. It can be easily proven that the partial trace yields the same result irrespective of the employed basis of A.

Its relation with measurements is the following one. The partial trace of M on the pure state  $|\Psi(T)\rangle_{MS}\langle\Psi(T)|_{MS}$  of equations (6),(7), under the effective "collapse" conditions for  $g,T,\sigma$ , precisely yields the unconditional post-measurement density matrix of equation (8). The same happens in any generalized measurement: the partial trace of A in  $U_{AS} |\theta\rangle_A \otimes |\psi\rangle$  will yield the unconditional post-measurement density matrix  $\hat{\rho}_S = \sum_m |\psi_m\rangle_S \langle \psi_m|_S$ . In general, this indicates that the partial trace of an ancilla partition A of a composite Hilbert space  $A \otimes S$  can always be interpreted as how the S would be left if an unconditional ideal projective measurement was performed on the A [11]. Note very importantly that if the traced out partition is not projectively measured (coupling a measurement ancilla to it and evolving until macroscopic distinguish-ability is achieved) and the interaction between A and S is not "thermalised" or does not cease indeterminately, then the reduced density matrix of S will just be a "fiction", that will not evolve independently of A, as does happen in the case of a real measurement. Each CWF of the S for different A states (which we placed in different slots of the matrix after partial tracing) will still interact with each other since they are not EWF-s. Yet, it is still true that for statistical measurement predictions about the S, the information in the reduced density matrix will be enough. Thus, under Bohmian mechanics, the reduced density matrix is in general just a "ficticious" "how the S would be left if", useful to predict single-time measurement statistics on S.

In order to finish integrating the density matrix formalism and any general quantum operation (including the generalized measurements) with this Bohmian view, we can invoke the Gelfand-Naimark-Segal theorem [12, 11]. By this theorem, we can assure that for any most general operation we can perform on a density matrix  $\hat{\rho}_S$  of a system S (any complete-positive, convex linear and not trace increasing superoperator acting on S), say, for the operation  $\mathfrak{S}$ , there exists at least an ancilla system A with a pure state  $|\theta\rangle_A$  and a coupling unitary evolution  $\hat{U}_{AS}$  such that:

$$\mathfrak{S}[\hat{\rho}_S] = tr_A \left[ (\hat{\Pi}_A \otimes \hat{I}d_S) \hat{U}_{AS} (|\theta\rangle_A \langle \theta|_A \otimes \hat{\rho}_S) \hat{U}_{AS}^{\dagger} \right]$$
(9)

which can be interpreted as a unitary coupling of the initially independent S and A, and posterior partially unconditional ideal projective measurement of A (where only the eigenstates of non-null eigenvalue of  $\hat{\Pi}_A$  are left and the rest are discarded). In particular, if the coupling of S and A perfectly entangles the eigenstates of  $\hat{\Pi}_A$  with some orthonormal basis of S, this will be a projective measurement of S. Else, it will be a generalized measurement of S. In the trivial case where  $\hat{U}_{AS} = \hat{U}_A \otimes \hat{U}_S$  and  $\hat{\Pi}_A = |\theta\rangle_A$ , it will just be the Schrödinger unitary evolution of S.

## Markovian to Non-Markovian Open Quantum Systems

Following the Markovianity idea we pragmatically defined earlier, we could call a Markovian open quantum system, any evolution of the reduced density of the S that could be equivalently interpreted as if a different portion of the environment (a different ancilla) instantly got coupled every  $\Delta t$  with the S and was then ideally measured, in a way that this ancilla never again interacted with the system (or their entanglement was somehow "thermalised" before their next interaction) [15]. This is equivalent to a generalized measurement of S every  $\Delta t$ . Among others, the "Past-Future Independence" definition of Markovianity by Wiseman  $et\ al.\ [14]$ , perfectly matches this view.

In fact, as shown by Ref [13], such a continuous monitorization of different ancillas that get coupled to the system at each time, can be used to derive some dynamical equations for the reduced density matrix of a subsystem in a Markovian environment, a type of so called Lindblad master equations [11, 14]. Then the generalized derivation of an arbitrary Markovian environment Lindblad master equation, requires the consideration of several simultaneous continuous measurements for different properties of the bath [13, 14], which still follows the same idea.

The fact that the dynamics of the reduced density matrix of a subsystem can be understood in these terms means that instead of trying to solve the Markovian master equation, we could do the following. Find an observable W for some (fictitious or not) environment ancillas, E, ancillas that get entangled with S and are then projectively measured, producing the same average (unconditional) effect on the reduced density of S as the predicted one by the master equation (which is always possible for a Markovian E sa said). Then, we could evolve a pure state-vector of the S choosing at each projective measurement of the bath, one of the possible stochastic conditional states. This would generate a linked in time S pure state  $|\psi_{w(t)}(t)\rangle_S$ , associated to the result of a certain continuous measurement (or unravelling) of the bath ancillas:  $w(t)^6$ . This pure state is called a **quantum trajectory**, linked to a "noise realization" w(t) for its environment [11, 14, 15]. As we saw previously that the reduced density matrix of a subsystem is how it would be left if an unconditional ideal measurement was performed on the rest of the system, this tells us that we should be able to recover the reduced density for the S by averaging the ensemble of all possible quantum trajectories for the unraveling of the W observable of the bath ancillas [14, 15]:

$$\hat{\rho}_S(t) := tr_{ES}[\hat{\rho}_{ES}(t)] = \mathbb{E}_{w(t)} \left[ \left| \psi_{w(t)}(t) \right\rangle_S \left\langle \psi_{w(t)}(t) \right|_S \right]$$
(10)

<sup>&</sup>lt;sup>6</sup>Remember that at each time a different generalized measurement is performed on S, meaning this stochastic trajectory w(t) reflects the Bohmian positions of different measurement dials at each  $\Delta t$  step. Thus, its non-differentiable nature is not a problem for Bohmian mechanics.

Computationally, this means that if we got an equation ruling the stochastic time evolution of a pure quantum trajectory  $|\psi_{w(t)}\rangle_S$  and its noise realization w(t), we would be able to compute in parallel the density matrix using simpler data structures (vectors) [14, 15]. Additionally, the obtained reduced density matrix is necessarily positive definite by construction. Equations of these kind are the so called, **Stochastic Schrödinger Equations** (SSE-s) [11, 13]. Note that such a pure state trajectory for a Markovian E, can always be physically interpreted in the Orthodox explanation, as a so called pure unravelling [14] (where one would invoke the collapse at each  $\Delta t$ ). In the Bohmian view a quantum trajectory is exactly a normalized CWF of the S (in ket notation), which every significant  $\Delta t$  is converted into an EWF (thus the normalization).

However, what if we had an E that gets entangled with the S, but which never really allows us to consider an effective collapse? What if the different CWF-s of the S, were allowed to interact in any future time, and were not converted into EFW-s every  $\Delta t$ ? That is, what if the "quantum trajectories" could interact between them, such that the evolution of each of them depended on the rest? Then "the information leaked" onto the environment from S (the "empty waves"), would be able to affect back S in any significant future time for S. Such an environment with "memory" of the entanglement achieved with S could be called a non-Markovian environment [14]. Then, it turns out that from a Bohmian interpretation, we could still continue talking about "pure state quantum trajectories", which would be the CWF-s for the S (in any desired representation), conditioned on a position for the environment interacting with S (or conditioned on the position of a dial coupled with an arbitrary observable of the E interacting with the S) [17, 16]. Since measurement and collapse are just described as another unitary evolution of the whole, and the positions are ontologically real at all times, then there is no interpretative issue.

Contrarily, in the Orthodox view, a CWF (normalized or not and in any representation basis), does not have a physical interpretation, unless it is an EWF, say, unless the conditioning variable is projectively measured. As a consequence, if a SSE is found for a non-Markovian dynamical equation ruling a reduced density matrix, the conditional pure state evolved by the SSE in the Orthodox view can only be understood as the state in which S would be left on, if the E was measured...but since it is non-Markovian, we cannot assume the E is being projectively measured! If it was, the evolution of the state would be pretty different (we would neglect part of the quantum wholeness, the interaction between the CWF-s stacked along the E axes). Thus, the linking of such states in time, can only be understood if we get out of the Orthodox and use concepts like the CWF of the Bohmian view [17, 16]. Of course, mathematically, one could derive such non-Markovian SSEs as pragmatical computational tools to reconstruct the reduced density matrix, but one would need to avoid any additional consideration for the quantum trajectory (like two-time correlation computations) unless one accepts some sort of ontological reality (independent of measurement) for the conditioning property of the environment.

From the Bohmian perspective it is easy to notice why SSE-s for non-Markovian environments will not be exact in general. One of the main properties a SSE needs to have is that it should allow the time evolution of a single conditional state independently of the rest of possible conditional states. This is precisely to ask that there is no quantum influence between adjacent CWF-s, influence which as explained in the beginning, is the main signature of quantum mechanics (the quantum wholeness). In fact, this is asking for these CWF-s to be EWF-s as we saw, which would then allow a Markovian interpretation for the SSE, and thus would imply a contradiction. Yet, SSEs that approximate the dynamics for ad-hoc cases are indeed possible in non-Markovian environments [18, 19, 6]. This is because, an ensemble of CWF-s does not need to be an ensemble of EWF-s to allow the computation of the reduced density matrix at each time!

To see that this is so, independently of the nature of the environment, let us prove it for an arbitrary composed pure state (the generalization to mixed states is then trivial). Given the arbitrary state  $|\Psi\rangle_{ES}$  for the environment E and system S, with position observables  $\vec{y}$  and  $\vec{x}$  respectively, just as

<sup>&</sup>lt;sup>7</sup>In fact, a whole set of CWF-s, if the system state was not mixed, would also allow the reconstruction of the full wavefunction! In which case a reduced density matrix would not even be necessary.

introduced in the beginning<sup>8</sup>:

$$|\Psi(t)\rangle_{AS} = \int \left|\vec{y}^{\xi}(t)\right\rangle_{A} \otimes \left|\psi^{\xi}(t)\right\rangle_{S} d\xi = \int \left|\vec{y}\right\rangle_{A} \otimes \left|\psi^{y(\xi,t)}(t)\right\rangle_{S} dy \tag{11}$$

Then tracing out A in  $\hat{\rho}_{AS}(t) = |\Psi(t)\rangle_{AS} \langle \Psi(t)|_{AS}$ , we would get the reduced density for the S:

$$tr_{E}[\hat{\rho}_{AS}(t)] = \int \langle \vec{y} | \hat{\rho}_{AS}(t) | \vec{y} \rangle dy = \int \left| \psi^{y(\xi,t)}(t) \right\rangle \left\langle \psi^{y(\xi,t)}(t) \right| dy = \mathbb{E}_{y(\xi,t)} \left[ \left| \psi^{y(\xi,t)}(t) \right\rangle \left\langle \psi^{y(\xi,t)}(t) \right| \right]$$

$$(12)$$

Which proves the ensemble average of the CWF-s reproduces the reduced density.

This clear narrative in terms of Bohmian CWF-s for non-Markovian open quantum systems is not only theoretically insightful, but is a **practical** tool to look for reasonable SSE-s. To exemplify this, let us describe two practical frameworks we developed.

## Non-Markovian SSE for two-terminal electronic devices operating at THz frequencies

Following Bohmian mechanics and Ref.[8], we have already shown after equation (3), a way to obtain SSE-s for arbitrary settings. In principle, in those equations the CWF of the S and the E are coupled at all times, not only between them, but also with the rest of possible CWF-s (non-Markovianity). However, for specific scenarios, we can make educated guesses for the quantum correlation terms G and J, and the classical potential U, to render a SSE for individual CWF-s of the S.

For nano-scale electronic devices operating at very high frequencies (in the order of THz), both the relevant dynamics of the S and the measurement coupling times are below picoseconds time-scales, implying Markovian assumptions for environment coupling are meaningless: there is "no time for their entanglement to be forgotten" [6]. This problem for a two-terminal nano-electron device is approximated in the BITLLES simulator [20, 21, 6], as an application example of the mentioned method. For this, the classical potential is evaluated as the solution of the Poisson equation [21], while G and J are modeled by a proper injection model [22] as well as proper boundary conditions [23, 24] that include the correlations between the active region of the two-terminal nano-device and the reservoirs. Even electron-phonon decoherence effects can be included effectively [25].

The electrons contributing to the electrical current, the observable of interest, are mainly the n/3 electrons in the active region of such a nano-device, thus we consider the active region is the subsystem S of interest. The number n/3 fluctuates in time as there are electrons entering and leaving this region. Such a "creation and destruction" of electrons, from the point of view of S, leads to an abrupt change in the degrees of freedom of its CWF. This problem can be circumvented in Bohmian mechanics by decomposing the CWF of S,  $\psi^{\xi}(\vec{x},t)$ , into a set of CWF-s for each electron. That is, for each of the n/3 electrons of position  $\vec{x}_k := (x_{3k+1}, x_{3k+2}, x_{3k+3})$  with  $k \in \{0, ..., n/3 - 1\}$ , we define a single particle CWF  $\phi_k^{\xi}(\vec{x}_k,t) := \psi^{\xi}(\vec{x}_k,\vec{x}_{\neg k} = \vec{x}_{\neg k}^{\xi}(t),t)$  with  $\vec{x}_{\neg k} = (\vec{x}_1,...,\vec{x}_{k-1},\vec{x}_{k+1},...,\vec{x}_{n/3})$ . Then, we can consider a set of n(t)/3 equations like (3), one for each of the electrons, to evolve each  $\phi_k^{\xi}$ . Note that what we have just done is to consider S, the subsystem of the non-Markovian open quantum system, as itself composed of several open quantum systems that will interact with each other in a non-Markovian way.

Now, the active region of the electron device S, is connected by a macroscopic cable (representing the portion of the environment A that gets entangled with the S) to an ammeter (acting as a measuring apparatus M). The electrical current read by the Bohmian position of the dial in the ammeter is the observable we want to predict. Thus, in principle the evaluation of the electrical current should require keeping track of all the environment degrees of freedom. However, it is known that the total current

<sup>&</sup>lt;sup>8</sup>Note that since Bohmian trajectories do not cross each other in configuration space, if we sampled only Bohmian trajectories for which  $\vec{x}(0)$  is a single position  $\vec{a}$ , at each time, we would still have a CWF per each position in  $\vec{y}$ . Thus, we have that the states  $\left\{\left|\psi^{y(\xi,t)}(t)\right\rangle_S:=\left\langle y(\xi,t)\right|_A\left|\Psi(t)\right\rangle_{AS}\mid\vec{x}(0)=\vec{a}\right\}_{y\in\mathbb{R}^{N-n}}$  are all the possible slices of the  $\vec{y}$  axis.

density, defined as the sum of the particle and displacement currents, is a divergenceless vector [26, 27], which makes the total current evaluated at the ends of the active region be equal to the total current evaluated at the cables. It is additionally known [28] that since the cable, unlike the active region, has macroscopic dimensions, the current at the ends of the active region is only due to the electrons in the active region (plus a nearly white noise). This is qualitatively because the electrons in the metallic cables have a very short screening time, meaning the electric field generated by an electron in the cable spatially decreases rapidly due to the presence of many other mobile charge carriers in the cable that screen it out. Thus, the contribution of these outer electrons to the displacement current at the border of the active region is negligible [30]. Therefore, the variable of the environment associated to the total current  $z(t) \equiv I(t)$  can indeed be equivalently computed at the boundary of the S. Finally, such a current (its expected value), can be computed from the Bohmian trajectories of the electrons in the active region as we will later explain.

In Ref. [6] we provide some numerical results demonstrating the ability of the presented method, by simulating a two-terminal electron device whose active region is a graphene sheet, contacted to the outer by two (ohmic) contacts. Here, to further take into account the electromagnetic environment of the electron device, we model the interaction between the graphene device and the environment through a resistor and a capacitor in series. The details are found in the mentioned article.

## Towards another general framework to look for position SSEs

We have developed a second framework to look for SSEs (equations to evolve CWF-s independently), based on the Born-Huang ansatz of the full wavefunction, at the cost of having a suitable guess for the conditional energy eigenstates of the relevant parts of the environment. For this, given the full, subsystem-environment Hamiltonian  $\hat{H}(\vec{x}, \vec{y}, t) = \sum_{k=1}^{N} \frac{-\hbar^2}{2m_k} \frac{\partial^2}{\partial x_k^2} + U(\vec{x}, \vec{y}, t) + V(\vec{x}, t)$ , we can define the transversal section Hamiltonian as  $\hat{H}_x(\vec{y}, t) := \sum_{k=m+1}^{N} \frac{-\hbar^2}{2m_k} \frac{\partial^2}{\partial x_k^2} + U(\vec{x}, \vec{y}, t)$ . Then, we define the set of eigenstates  $\{\Phi_x^j(\vec{y}, t)\}_j$  with eigenvalues  $\{\varepsilon_x^j(t)\}_j$ , parametrized by the chosen section  $\vec{x}$ , to be the solution of:  $\hat{H}_x(\vec{y}, t)\Phi_x^j(\vec{y}, t) = \varepsilon_x^j(t)\Phi_x^j(\vec{y}, t)$ . We call these states  $\Phi_x^j(\vec{y}, t)$ , the transversal section eigenstates (TSE). Since the hermiticity of the operator  $\hat{H}_x(\vec{y}, t)$  implies the TSE-s form an orthonormal basis for the Hilbert space of  $\vec{y}$  at each  $\vec{x}$ , we could expand the following ansatz:  $\Psi(\vec{x}, \vec{y}, t) = \sum_j \Lambda^j(\vec{x}, t)\Phi_x^j(\vec{y}, t) = \sum_j \varphi_j(\vec{x}, \vec{y}, t)$ , with  $\Lambda^j(\vec{x}, t) := \int \Phi_x^j(\vec{y}, t)\Psi(\vec{x}, \vec{y}, t)dy$  the projection coefficients and  $\varphi_j(\vec{x}, \vec{y}, t) := \Lambda^j(\vec{x}, t)\Phi_x^j(\vec{y}, t)$ .

Now, using this expansion in the Schrödinger Equation, and evaluating the full wavefunction along the trajectory for the environment  $\vec{y} = \vec{y}^{\xi}(t)^{10}$ , we can get by denoting  $\varphi_{\xi}^{k}(\vec{x},t) := \varphi^{k}(\vec{x},\vec{y}^{\xi}(t),t)$  that:

$$i\hbar \frac{\partial}{\partial t} \varphi_{\xi}^{k}(\vec{x}, t) = \left[ -\sum_{s=1}^{m} \frac{\hbar^{2}}{2m_{s}} \frac{\partial^{2}}{\partial x_{s}^{2}} + \varepsilon^{k}(\vec{x}, t) + V(\vec{x}, t) + i\hbar \frac{\mathrm{d}}{\mathrm{d}t} log(\Phi_{x}^{k}(\vec{y}^{\xi}(t), t)) \right] \varphi_{\xi}^{k}(\vec{x}, t) + (13)$$

$$+\sum_{j=0}^{\infty}\sum_{s=1}^{m}\frac{-\hbar}{2m_{s}}\Biggl(\frac{1}{\Phi_{x}^{j}(\vec{y}^{\xi}(t),t)}\frac{\partial^{2}\Phi_{x}^{j}(\vec{y}^{\xi}(t),t)}{\partial x_{s}^{2}}+2\frac{\partial}{\partial x_{s}}log(\Phi_{x}^{j}(\vec{y}^{\xi}(t),t))\Biggl[\frac{\partial}{\partial x_{s}}-\frac{\partial}{\partial x_{s}}log(\Phi_{x}^{j}(\vec{y}^{\xi}(t),t))\Biggr]\Biggr)\varphi_{\xi}^{j}(\vec{x},t)$$

Because the CWF for the subsystem can be recovered from  $\psi^{\xi}(\vec{x},t) = \sum_{j} \varphi_{\xi}^{j}(\vec{x},t)$ , we have obtained a set of exact linear equations involving only n dimensional states (instead of N) that allow the evolution of single CWF-s. In principle, since a general Hilbert space will need to have a countably infinite number of orthonormal states in a basis, it would be a set of infinite number of equations.

<sup>&</sup>lt;sup>9</sup>The classical potentials are allowed to have a time dependence to account for classical interaction with the rest of the environment.

<sup>&</sup>lt;sup>10</sup>In reality, we could choose any trajectory we like for the environment if we are not interested in computing Bohmian trajectories. Thus, it could be the result of a measurement of the environment, or just a set of trajectories that leads us to the reconstruction of the reduced density with the least number of them.

However, we shall reasonably truncate the expansion of the CWF at a relatively low fixed point (at which for example the norm of the CWF surpasses a certain threshold), or even allow it to vary in time. If so, the difficulty of these equations would only relay on the knowledge of the TSE-s  $\Phi_x^j(\vec{y},t)$ . The point is that providing educated guesses for them seems to be more reasonable than guessing for G and J, and might be a starting point for the derivation of ad hoc SSE-s for particular non-Markovian environments.

## Can we predict all observables using Bohmian trajectories?

From the provided narrative, we can see that a measurement operator  $\hat{G} = \sum_{g} g |g\rangle \langle g|$ , is just a way to gather an orthonormal basis  $\{|g\rangle\}_g$ , where each  $|g\rangle$  is linked with a value g. We also saw that a projective measurement that uses G in its interaction Hamiltonian, reveals the **post**-measurement state  $|q\rangle$ , as a function of the measured q, which will happen with a probability due to the **pre**measurement state. With enough repetitions, we could end up knowing these probabilities, which are related to the projection of the pre-measurement state onto the possible post-measurement states. Beyond serving to reveal the post-measurement state and pre-measurement state's projection coefficients, in the provided Bohmian view, the measured value g related to  $\hat{G}$ , is devoid of any additional meaning (unless  $\hat{G}$  is a function of the position operator, in which case we say q is the **post**measurement property of a Bohmian trajectory). But then, in general, is this q (say for a momentum, an energy or a spin measurement) just a mathematical tool? That is, we cannot say g is a property of the wavefunction, since otherwise we would need to say that a state in superposition has multiple simultaneous observable values. But apparently, we cannot either say in general, it is a property of the Bohmian trajectory, and when we can say so, it is just a post-measurement S property. However, if "measuring" as Bell said [31], is about revealing information of the unmeasured (pre-measurement) system: are the projection probabilities of the wavefunction the only thing we can really know about the unmeasured system? All these questions were not experimentally interesting until recently the community acknowledged that some properties predicted for unmeasured S Bohmian trajectories could indeed be experimentally measured, when Wiseman proposed his protocol to operationally measure the Bohmian velocity of a pre-measurement system [32].

More recently, some of the authors derived a striking observation that extends this concept, allowing, if wished, not only to derive an Orthodox observable operator for any property of a Bohmian trajectory, but to consider that any Orthodox observable operator (even the ones not commuting with the position operator), can always be understood as an observable property of the Bohmian trajectory, meaning this g can indeed be always understood as a well defined property of a trajectory [34, 35]. Not only that, but, no matter if we consider this identification a simple mathematical tool, it leads to several **practical** advantages in the characterization of a quantum system, because in fact, their "pre-measurement" value for any system can indeed be measured.

Given any arbitrary (Hermitian) operator  $\hat{G}$ , describing the observable property G for the subsystem S, with normalized EWF  $|\psi(t)\rangle$ , let us define the function  $G^{\psi}(x,t) := \frac{\langle \vec{x}|\hat{G}|\psi(t)\rangle}{\langle \vec{x}|\psi(t)\rangle}$  (which as will be discussed later on, is the weak value [33] of  $\hat{G}$  for the state  $|\psi(t)\rangle$  at time t, post-selected at  $\vec{x}$ ). Then, we could define a real function  $G_B^{\psi}(\vec{x},t) = \mathbb{R}e\{G^{\psi}(x,t)\}$ , which we say is the property G of the Bohmian trajectory passing from  $\vec{x}$  at time t. Until here it seems just a cumbersome definition. Yet, let us compute the expected value for  $\hat{G}$  and try to write it as a function of  $G^{\psi}(x,t)$ :

$$\langle \hat{G} \rangle(t) = \langle \psi(t) | \hat{G} | \psi(t) \rangle = \int \langle \psi(t) | | \vec{x} \rangle \langle \vec{x} | \hat{G} | \psi(t) \rangle dx = \int |\psi(\vec{x}, t)|^2 G^{\psi}(\vec{x}, t) dx \tag{14}$$

which means that the spatial average of the (possibly complex)  $G^{\psi}(x,t)$ , gives the same expected value for the observable G as using the operator  $\hat{G}$ . But here comes the most interesting point: since  $\hat{G}$  is an observable, its expected value will be a real number, meaning that  $\langle \hat{G} \rangle = \mathbb{R}e\{\langle \hat{G} \rangle\}$ , which means:

$$\langle \hat{G} \rangle(t) = \int |\psi(\vec{x}, t)|^2 G_B^{\psi}(\vec{x}, t) dx = \lim_{|\Sigma| \to \infty} \frac{1}{|\Sigma|} \sum_{\xi \in \Sigma} G_B^{\psi}(\vec{x}^{\xi}(t), t)$$
 (15)

where we additionally used the quantum equilibrium hypothesis [7] for the set of trajectories  $\{\vec{x}^{\xi}(t)\}_{\xi\in\Sigma}$  sampled in independent repetitions of the experiment. This equation means that the real property  $G_B^{\psi}(\vec{x}(\vec{\xi},t),t)$  of the  $\vec{\xi}$ -th Bohmian trajectory, averaged over the ensemble of possible trajectories, gives the same value as the operator's expected value. Still,  $G_B^{\psi}$  could be nothing more than an ad-hoc definition for this to be satisfied. The true hit though, comes with the following: what would the suggested Bohmian property related with G be if the system state  $|g\rangle$ , was an eigenstate of  $\hat{G}$  with eigenvalue g?

 $G_B^{\psi}(x) = \mathbb{R}e\left\{\frac{\langle \vec{x}|\,\hat{G}\,|g\rangle}{\langle \vec{x}|g\rangle}\right\} = \mathbb{R}e\left\{\frac{\langle \vec{x}|\psi\rangle\,g}{\langle \vec{x}|\psi\rangle}\right\} = g \tag{16}$ 

This suggests  $|g\rangle$  is an eigenstate of  $\hat{G}$  if and only if it is a state for which every Bohmian trajectory has the same value of the property G. The implications of this are twofold. First, this says that effectively, the measured g in a projective measurement, is indeed a property of the Bohmian trajectory (if we wish). Second, this is then a tool to construct the operator  $\hat{G}$  itself, by defining  $\hat{G}$  in terms of  $G_B^{\psi}$ . We could define  $\hat{G}$  as the collection of states in which all Bohmian trajectories have the same value g for  $G_B^{\psi}$ . This is useful for there are observables, like the many electron current in a nano-device, for which there is no clear measurement operator, but there is a clear Bohmian observable associated with it [29, 28], as we will see.

As the icing of the cake, it turns out, as we proved in [34], that if we set as  $\hat{G}$ , the momentum operator  $\hat{p}_k$  of the k-th degree of freedom, the Bohmian trajectory property  $G_B^{\psi}(\vec{x},t)$  is exactly equal to the Bohmian momentum of the trajectory crossing  $\vec{x}$ :  $m_k v_k(\vec{x},t)$ . If we set as  $\hat{G}$ , the Hamiltonian operator  $\hat{H}$ , the property  $G_B^{\psi}(\vec{x},t)$  turns out to be exactly equal to the Bohmian energy (kinetic plus classical and quantum potentials [5]) of the trajectory crossing  $\vec{x}$ . And the list of these "fortunate" matches goes on. Even beyond. For instance, if wished, we could have at all times a simultaneous deterministic value for the three components of spin [36].

In summary, since we placed no restriction on  $\hat{G}$ , this means that for **every** observable of a quantum system, we are mathematically safe (if wished), to assume that at all times, each Bohmian trajectory has an ontologically determined value for all of them. Moreover, these values will in fact evolve continuously in time, as long as wavefunctions always evolve so. This has yet another striking consequence: if g is the observed value for a trajectory after a von Neumann coupling (thus the value we measure strongly), and the trajectory had another value for G before the interaction started, then the property G took all intermediate values before taking g, not necessarily among the eigenvalues of  $\hat{G}$ . Thus, if we want, we are safe to see the "quantization" of quantum mechanics as an apparent property, due to the fact that for a "proper" measurement, we require that a dial saying g is compatible with a wavefunction  $|g\rangle$  that will give a measurement g with probability 1. That is, a wavefunction which has all its Bohmian trajectories with value g for G. Then, we simply call it "quantum" because this delicate orchestration can only happen for a certain "quantized number" of states.

As if all this was not already hard to digest, there is even an additional point to be remarked. If we could only measure  $G_B^{\psi}$  when we forced it, by a von Neumann interaction, to be an eigenvalue of  $\hat{G}$ , all this would have no practical application. However, it turns out, we can actually measure the "unmeasured"  $G_B^{\psi}$  for **any** Bohmian trajectory. The "how", explains the "cumbersome" definition. We defined  $G_B^{\psi}$  as the real part of a weak value, a particular one we have named the "local-in-position weak value" [34, 35]. As it is well known [33], the real part of a weak value can indeed be experimentally measured. For this, first we couple an ancilla to the subsystem of EWF  $|\psi\rangle$ , through a von Neumann Hamiltonian  $\mu(t)\hat{p}_A\otimes\hat{G}$  (which produces a separation in macroscopically separated eigenstates of  $\hat{G}$  if coupled with a big enough interaction strength  $\mu$ ). Let the interaction strength be very small, such that the system state is only slightly perturbed (just a little amount of information is leaked to the ancilla). Now strongly measure the slightly entangled ancilla's position (through a strong coupling of a second ancilla, etc.). This will yield a weak measurement about  $\hat{G}$  for the S. Note the von Neumann Hamiltonian is such that no matter the strength  $\mu$ , the position of the ancilla will always have the same expected value as the coupled observable (in our case G). There is still a step more though. Right

after the weak measurement of G has been performed, a third ancilla is rapidly coupled to the (only slightly perturbed) S, with a Hamiltonian to projectively measure the position of the S(according to the Bohmian view, this position is in fact the Bohmian position of the system). Finally, we average the weak measurements that after-wards lead us to measure the system position at a fixed  $\vec{x}$ . The result will be exactly  $G_B^{\psi}(\vec{x},t)$  [33, 34]. One could legitimately say, this is just juggling with numbers due to several observations. But, one could also perfectly legitimately say (especially after what we have revealed) that the average weak measurements of G, for experiments in which the system was at  $\vec{x}$ , gave  $G_B^{\psi}(\vec{x},t)$ , because all the times that our Bohmian trajectory was at  $\vec{x}$ , the system had indeed the property  $G_B^{\psi}(\vec{x})$ . Phenomenologically this assertion is of course unprovable, yet, in the operational sense mentioned by Ref. [32], it seems to be a simpler view for a pragmatic experimentalist.

### Practical Applications of Local-In-Position Weak Values

This Bohmian discovery, as already anticipated, has several practical applications [34, 35]. On the one hand, we can numerically predict the expected value for an observable without the need to have explicitly defined its formal operator. One can derive the observable  $G_B^{\psi}(x,t)$  in the language of Bohmian mechanics, which is very akin to classical mechanics, and compute the ensemble average of the property to get the expected value of the operator related to it. For example, this is how we can predict the total electrical current crossing the active region of a two-terminal nano-device operating at high frequencies (THz) [28, 29]. The total current at such frequencies needs to consider the displacement operator  $\hat{I}$  should look like. However, we can define the current due to the Bohmian trajectory of a k-th electron  $\vec{x}_k^{\xi}(t)$  of charge q through a surface  $\sigma$  as:  $I_k^{\xi}(t) = \int_{\sigma} \vec{J}^{\xi}(\vec{r},t) \cdot d\vec{s} + \int_{\sigma} \varepsilon(\vec{r},t) \frac{\partial \vec{E}^{\xi}(\vec{r},t)}{\partial t} \cdot d\vec{s}$ , where  $\varepsilon(\vec{r},t)$  is the electric permittivity ,  $\vec{J}^{\xi}(\vec{r},t) = q \frac{d\vec{x}_k^{\xi}(t)}{dt} \delta(\vec{r} - \vec{x}_k^{\xi}(t))$  is the particle current density, and  $\vec{E}^{\xi}(\vec{r},t)$  is the electric field generated by the electron, as a solution to the Gauss equation. Then, as proven in [29], for two terminal devices of longitudinal length L with metallic contact surfaces  $\sigma$  of width and height w, h >> L, the total current contribution in these surfaces is:  $I_k^{\xi}(t) = \frac{q}{L}v_k^{\xi}(\vec{x} = \vec{x}_k(t),t)$ , where  $v_x$  is the longitudinal Bohmian velocity of the electron. The total Bohmian current at the surface  $\sigma$  will then be the sum of these contributions  $I^{\xi}(t) = \sum_k I_k^{\xi}(t)$ , such that  $\mathbb{E}_{\xi}[I^{\xi}(t)] = \langle \hat{I} \rangle(t)$ .

As a second and perhaps the most sounded application led by this discovery: it provides an operational answer to the search of non-contextuality in the definitions of measurements involving two different times [34]. Saying that a property of a system is contextual means that its value depends on the environment employed to convey that information to the observer, that it is not an "unmeasured system" property. Several considerations arise here:

(1.) We can measure a single-time (static) expectation of a property G for the S,  $\langle \hat{G} \rangle$ , averaging the results of several quantum measurements. Which-ever fiducial state we employ in an either strong or weak measurement, the result will be the same and equal to the expectation calculable by only knowing the pre-measurement EWF of the S (thus it is a measurable non-contextual property of the S). However, it will not be as easy if we want to know the expectation of the product of two observables (time correlation), between an observable F at time  $t_1$  and any observable G at time  $t_2$ . Especially if we need this information to contain exclusively information about the unmeasured S. We could correlate the result of a strong measurement of F at time  $t_1$  and a strong measurement of G at time G0, but since the measurement at G1 will project the state to different EWF-s, the backaction of the measuring device will be obvious. In fact, even numerically it seems hard to be well defined. If their operators do not commute,  $\langle \hat{G}(t_2)\hat{F}(t_1) \rangle$ , in the Heisenberg formalism, will give a complex number in general. Alternatively, we could look for  $\mathbb{R}e\left\{\langle \hat{G}(t_2)\hat{F}(t_1) \rangle\right\}$  which would now be real and turns out to be the correlation of a weak measurement of G1 at time G2 (thus, also experimentally measurable). In addition it seems to provide a "backaction-free" correlation

<sup>&</sup>lt;sup>11</sup>The legitimacy of a well defined electric field in Bohmian mechanics will be described in the last part of the chapter.

definition for the dynamic variables. Yet, as shown in [36], even an ideally weak measurement does in fact perturb the system in a way that is dependent, for example, on the particular fiducial state employed for it.

- (2.) Since work is a dynamical property implying at least two times, this contextuality issue has led in quantum thermodynamics to a "no-go" theorem [37] stating that there cannot exist a work superoperator that simultaneously satisfies all the physical properties required from it. Other history dependent thermodynamic properties suffer from the same issue [38, 39]: a definition of them always seems to be dependent on a particular measuring scheme, which causes as many quantum work definitions as say, acceptable measurement fiducial states exist.
- (3.) A similar issue raises when trying to measure the maximum working frequency of state-of-the-art transistors to test the performance of modern computers [40]. For this, the time spent by electrons in the active region of such nano-scale transistors, their "dwell time", must be measured. One could place position detectors in the two ends of the active region, but this metric would be unsuitable since in operation, no computer has such detectors at the ends of its transistors [41, 42].

All these points call for a way to measure "unmeasured system" dynamical properties. Dynamical properties that could be predicted in a simulation without any explicit introduction of a particular measuring ancilla, but which could also be measured. It turns out, this is exactly what the found Bohmian property  $G_R^{\psi}(\vec{x},t)$  is.

(1.) As such, the problem of non-contextual two-time correlations of dynamical variables for a wavefunction  $|\psi(t)\rangle$ , can be circumvented by computing the expectation as would be done by a frequentist definition in a classical system. Given a big enough set of trajectories  $\{\vec{x}^{\xi}(t)\}_{\xi\in\Sigma}$  each with associated ontologically deterministic observables  $G_B^{\psi}(\vec{x},t)$  and  $F_B^{\psi}(\vec{x},t)$ , following quantum equilibrium [7] we could define:

$$\langle G(t_2)F(t_1)\rangle = \lim_{|\Sigma| \to \infty} \frac{1}{|\Sigma|} \sum_{\xi \in \Sigma} G_B^{\psi}(\vec{x}^{\xi}(t_2), t_2) F_B^{\psi}(\vec{x}^{\xi}(t_1), t_1) =$$
(17)

$$= \int |\psi(\vec{\xi},0)|^2 \, \mathbb{R}e \left[ \frac{\langle \vec{x}^{\xi}(t_2) | \hat{G} | \psi(t_2) \rangle}{\langle \vec{x}^{\xi}(t_2) | \psi(t_2) \rangle} \right] \mathbb{R}e \left[ \frac{\langle \vec{x}^{\xi}(t_1) | \hat{G} | \psi(t_1) \rangle}{\langle \vec{x}^{\xi}(t_1) | \psi(t_1) \rangle} \right] d\xi$$

(2.) In a similar way, we can solve the problems concerning a quantum work definition as done by [43, 44]. First note that given a general system Hamiltonian  $\hat{H} = \sum_{k} \frac{-\hbar^2}{2m_k} \frac{\partial^2}{\partial x_k^2} + V(\vec{x}, t)$ :

$$E_B^{\psi}(\vec{x}^{\xi}(t),t) = \mathbb{R}e\left[\frac{\langle \vec{x}^{\xi}(t) | \hat{H} | \psi(t) \rangle}{\langle \vec{x}^{\xi}(t) | \psi(t) \rangle}\right] = \sum_{k=1}^{n} \frac{1}{2} m_k v_k (\vec{x}^{\xi}(t),t)^2 + V(\vec{x}^{\xi}(t),t) + Q(\vec{x}^{\xi}(t),t)$$
(18)

with Q the well known Bohmian quantum potential [3, 4, 5]. This proves  $E_B^{\psi}(\vec{x}^{\xi}(t), t)$  is, as anticipated, the total Bohmian energy of the trajectory at time t. Then, following classical mechanics, we can compute its associated Bohmian work as the energy difference (if conservative, else employing an integral):  $W^{\xi}(t_1, t_2) = E_B^{\psi}(\vec{x}^{\xi}(t_2), t_2) - E_B^{\psi}(\vec{x}^{\xi}(t_1), t_1)$ . As a result, a non-contextual definition of the quantum work could be the ensemble average of the trajectory works:

$$\langle W(t_1, t_2) \rangle = \lim_{|\Sigma| \to \infty} \frac{1}{|\Sigma|} \sum_{\xi \in \Sigma} \left( E_B^{\psi}(\vec{x}^{\xi}(t_2), t_2) - E_B^{\psi}(\vec{x}^{\xi}(t_1), t_1) \right)$$

$$\tag{19}$$

(3.) Finally, we could give a reasonable Bohmian answer to the search of an "unmeasured" dwell time, as the expected time spent by the S Bohmian trajectory of the electron within the active region  $\Gamma \subset \mathbb{R}^3$ . Mathematically, the dwell time  $\tau$  for the  $\xi$ -th trajectory of the k-th electron with EWF  $\psi^{\xi}(\vec{x}_k,t)$  is by definition given by the Lebesgue integral:  $\tau_B^{\xi} = \int_0^{\infty} dt \int_{\Gamma} \delta(\vec{r} - \vec{x}_k^{\xi}(t)) dr$ . This makes the expected time  $\langle \tau \rangle$  be, by the quantum equilibrium hypothesis:

$$\langle \tau \rangle = \lim_{|\Sigma| \to \infty} \frac{1}{|\Sigma|} \sum_{\xi \in \Sigma} \tau_B^{\xi} = \int_0^\infty dt \int_{\Gamma} |\psi^{\xi}(\vec{r}, t)|^2 dr$$
 (20)

which turns out, is a well-known equation used to predict the dwell time.

Can we understand light matter interaction through well defined "Bohmian-electromagnetic fields"?

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