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Estimation of Piecewise-Deterministic Trajectories in a Quantum Optics Scenario

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The manipulation of individual copies of quantum systems is one of the most groundbreaking experimental discoveries in the field of quantum physics. On both an experimental and a theoretical level, it has been shown that the dynamics of a single copy of an open quantum system is a trajectory of a piecewise-deterministic process. To the best of our knowledge, this application field has not been explored by the literature in applied mathematics, from both probabilistic and statistical perspectives. The objective of this chapter is to provide a self-contained presentation of this kind of model, as well as its specificities in terms of observations scheme of the system, and a first attempt to deal with a statistical issue that arises in the quantum world.

I. INTRODUCTION

A. The postulates of Quantum Mechanics

Quantum mechanics is one of the most successful theoretical frameworks in physics, its predictions having been tested and verified with remarkable precision in countless scenarios. Roughly speaking, and with the due exceptions, quantum mechanics deals with phenomena happening at the sub-atomic, atomic and molecular scales, and with how these systems interact with one another. Several new and counterintuitive phenomena arise at these scales, such as non-locality [1], non-determinism [2], wave-particle duality [3], quantum entanglement [4], zero-point vacuum fluctuations [5] to name but a few. One key point, central in the quantum theory, is the fundamental and irreducible role played by measurements of a quantum system on the quantum system itself [3]. Quantum mechanics, rather than describing how a quantum system behaves in absolute terms, is in fact a theory of how a quantum system reacts when measured. This difference, which may appear almost semantic, is on the contrary of fundamental importance for the correct interpretation of the theory and lies at the core of many of the exotic phenomena observed in the quantum world. This bears two main consequences: first, on a practical level, the way measurements affect the observed system and the way the system interacts with its surroundings (thereby including the measuring apparatus) is an essential point in the structure of the theory; second, as suggested by the theory and verified by experiments, measuring does not simply reveal a property of a system but, instead, contributes in determining the property itself [6]. Quantum mechanics is thus an overcoming of classical mechanics but, at the same time, needs classical objects (measuring apparatus) for the appropriate definition of physical properties to associate to a system. This intricate tie between quantum and classical physics is probably the element that, more than others, make the interpretation of quantum mechanics a non-trivial task.

In the absence of an intuitive level of understanding, the mathematical structure of the theory is clear and well developed [7]. It rests on the following postulates, the ensemble of which is known as the Copenhagen interpretation of quantum mechanics.

Postulate 1 (System's state). The state of an isolated quantum system is described by a vector $|\psi\rangle$ in a complex projective Hilbert space \mathcal{H} . This vector contains the full information on any possible outcome of measurements performed on the system and, as such, represents the most complete description of the system's state. By definition of projective Hilbert spaces, state vectors have norm 1.

In the following we focus on the special but important case of systems whose Hilbert space is finite-dimensional.

Postulate 2 (System's properties). If the dimension of the system's Hilbert space is N , any measur-

able physical property \mathcal{A} on a system is represented by a Hermitian matrix A of dimension $N \times N$. Conversely, any $N \times N$ Hermitian matrix represents a measurable property on the system. Hermitian matrices are often referred to as observables. By the properties of Hermitian matrices, observables have real eigenvalues and orthonormal eigenvectors, forming a basis in the Hilbert space.

Postulate 3 (Measurement outcomes). The measurement outcome of an observable A on a system in the state $|\psi\rangle$ is a stochastic variable x . The support of x is the set \mathcal{E}_A of eigenvalues of A . For any $a \in \mathcal{E}_A$, being $|a\rangle$ the corresponding eigenvector, the probability function is given by $\mathbb{P}(x = a) = |\langle a|\psi\rangle|^2$, where $\langle v|u\rangle$ stands for the Hermitian inner product $\langle u, v\rangle$. In case of degeneracy, the probability is simply $\mathbb{P}(x = a) = \sum_i |\langle a_i|\psi\rangle|^2$, $\{|a_i\rangle\}$ being the subset of eigenvectors of A associated to eigenvalue a .

Postulate 3 is central in the interpretation of quantum theory as it specifies what kind of information the state vector provides and how this information can be experimentally accessed. The state vector is not directly measurable: what is measurable is the probabilistic structure it imposes to measurement outcomes.

Postulate 4 (Wave-function collapse). If property A is measured on a system in a state $|\psi\rangle$ yielding the outcome a , the state of the system changes **instantaneously** to the eigenstate $|a\rangle$ of A associated to the eigenvalue a . The discontinuous change $|\psi\rangle \rightarrow |a\rangle$ is referred to as wave-function collapse. In case of degeneracy the state after measurement collapses to $\frac{1}{\mathcal{N}} \sum_i c_{a_i} |a_i\rangle$, $\{|a_i\rangle\}$ being the subset of eigenvectors of A associated to eigenvalue a , c_{a_i} being the coefficient of $|a_i\rangle$ in the expansion of $|\psi\rangle$ on the basis of eigenvectors of A (see Postulate 2), and $\mathcal{N} = \sqrt{\sum_i |c_{a_i}|^2}$ is a normalization factor.

Postulate 5 (Time evolution). The state of an isolated system between measures evolves in time according to the so-called Schrödinger equation

$$\frac{d|\psi\rangle}{dt} = -\frac{i}{\hbar} H|\psi\rangle, \quad (1)$$

where $\hbar \simeq 1.05 \times 10^{-34} \text{ m}^2 \text{ kg s}^{-1}$ is the reduced Planck's constant and H , the system's Hamiltonian, is the observable of the energy of the system. For time-independent Hamiltonians, its formal solution is $|\psi(t)\rangle = U(t)|\psi(0)\rangle$, with the time-evolution operator $U(t) = e^{-\frac{i}{\hbar} Ht}$

B. Dynamics of open quantum Markovian systems

Subsection IA gave the basic postulates of quantum mechanics for isolated systems (with the exception of their interaction with measuring apparatus). However, in many situations of physical interest, the assumption of isolated systems breaks down due to the almost unavoidable coupling to the external world [8]. It is a matter of both theoretical interest and practical significance to extend the five postulates to the case of an open quantum system, i.e., a system S allowed to exchange energy and information with another system E , considered as an external environment. One can always imagine to identify E in such a way that the composite system $S + E$ can be regarded as isolated. The state of the total system is thus represented by a vector $|\psi_{SE}\rangle$. Under the assumption however of only having access to the subsystem S rather than to the global system $S + E$, the distribution of measurement outcomes on S will reflect at the same time the intrinsic probabilistic nature of quantum systems (Postulate 3) and our subjective lack of knowledge on the global system state due to our ignorance on E . Because information on the state of the system is only partial, the description of S in terms of a state vector (Postulate 1) does not hold anymore¹. To account for a

¹ This point of view, although useful in providing an intuition on the need of extending the structure of quantum mechanics to a new class of states, only gives a partial view: due to the existence of a specifically quantum kind of correlations between two systems

lack of knowledge about the specific vector state of a system S , a new class of quantum states needs to be introduced [9] describing statistical ensembles of vector states. Given a set of (not necessarily orthogonal) vectors $\{|\psi_i\rangle\}$, let us introduce the matrix

$$\rho = \sum_i w_i |\psi_i\rangle\langle\psi_i|, \quad (2)$$

with the weights $0 \leq w_i \leq 1$ and $\sum_i w_i = 1$. The notation $|u\rangle\langle v|$ stands for the complex outer product $u \otimes v^*$, v^* being the complex conjugate of v . By construction, ρ is a Hermitian matrix. In the case $w_k = 1$ for a certain k , the matrix (2) is referred to as a *pure state*, and *mixed state* otherwise. A mixed state represents a classical statistical mixture of pure states $|\psi_i\rangle\langle\psi_i|$, each contributing with a weight w_i . The 5 postulates of Subsection I A generalize to

Postulate 1b (Density matrices). The state of a (generally open) quantum system is described by a positive semidefinite Hermitian matrix ρ of the form (2) called its **density matrix**. The eigenvalues of this matrix are the probabilities that the system S be found in the corresponding eigenvector, which is a vector in the system's Hilbert space. This implies that $\text{Tr}\rho = 1$. A density matrix represents a pure state if and only if $\text{Tr}\rho^2 = 1$. A pure state is simply an alternative way of describing a vector state.

Postulate 2 does not change since it does not depend on the state of the system.

Postulate 3b (Measurement outcomes on density matrices). When measuring A on a state ρ , the probability of obtaining the specific eigenvalue a is $\mathbb{P}(x = a) = \langle a|\rho|a\rangle$. If ρ is a pure state $|\psi\rangle\langle\psi|$, $\mathbb{P}(x = a) = \langle a|\psi\rangle\langle\psi|a\rangle = |\langle a|\psi\rangle|^2$, as expected from Postulate 3. In the general case, one obtains $\mathbb{P}(x = a) = \sum_i w_i |\langle a|\psi_i\rangle|^2$, as expected from a statistical mixture of pure states.

Postulate 4b (Density matrix collapse). If the measurement of A on ρ yields the outcome a associated to the eigenvector $|a\rangle$, the density matrix instantaneously collapses to $\sigma_a = \frac{|a\rangle\langle a|\rho|a\rangle\langle a|}{\text{Tr}(|a\rangle\langle a|\rho|a\rangle\langle a|)}$

More in general, thereby including the case of degeneracy in the spectrum of observables, consider the spectral decomposition of $A = \sum_i a_i A_i$. Then $\mathbb{P}(x = a_i) = \text{Tr}(A_i \rho A_i)$ and $\sigma_{a_i} = \frac{A_i \rho A_i}{\text{Tr}(A_i \rho A_i)}$.

Postulate 5b (Density matrix evolution for closed systems). The Schrödinger equation, in the case of a closed system, generalizes to the von Neumann equation

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho], \quad (3)$$

with the commutator of two matrices $[A, B] = AB - BA$.

Extending postulate 5b to a generic open quantum system is generally not straightforward. Assuming the global system $S + E$ to be isolated, its pure state $\rho_{SE} = |\psi_{SE}\rangle\langle\psi_{SE}|$ evolves according to the von Neumann equation $\frac{d\rho_{SE}}{dt} = -\frac{i}{\hbar}[H_{SE}, \rho_{SE}]$, H_{SE} being the Hamiltonian of the global system, containing in general local Hamiltonians H_S and H_E of, respectively, S and E , and an interaction term V_{SE} . The density matrix ρ_S of subsystem S is obtained from ρ_{SE} by performing a partial trace $\text{Tr}_E \rho_{SE}$ over the degrees of freedom of E . One has, in general,

$$\frac{d\rho_S}{dt} = \frac{d\text{Tr}_E \rho_{SE}}{dt} = \text{Tr}_E \frac{d\rho_{SE}}{dt} = -\frac{i}{\hbar} \text{Tr}_E [H_{SE}, \rho_{SE}]. \quad (4)$$

The issue comes from the fact that no general way is known of obtaining a closed form for the r.h.s. of eq. (4), without any additional assumptions on the environment E and its interaction with

(entanglement), the state of a subsystem in a global entangled state cannot be described by a vector, even if full information on the global state is available. This aspect goes however beyond the scope of this brief overview.

S . However, in the case of weakly interacting systems and rapidly decaying correlation functions of E , the so-called Born-Markov approximation can be performed [9], which ultimately leads to a Markovian equation for the evolution of S (quantum master equation), which for an N -dimensional quantum system can always be cast in the so-called GKSL form as

$$\frac{d\rho_S}{dt} = -\frac{i}{\hbar}[\tilde{H}_S, \rho_S] + \sum_{i=1}^{N^2-1} \gamma_i \left(L_i \rho_S L_i^\dagger - \frac{1}{2} \{L_i^\dagger L_i, \rho_S\} \right). \quad (5)$$

Here \tilde{H}_S is the system's Hamiltonian, modified to take into account the change in the system's energy due to its interaction with E . The first term on the r.h.s. accounts for the free dynamics of S , not triggered by its interaction with E . The second term on the r.h.s., on the contrary, describes the dynamics of S directly induced by its interaction with E : L_i (Lindblad operators) are non-Hermitian matrices (L_i^\dagger stands here for Hermitian conjugation), each describing a specific dynamical process in S triggered by E and happening at a rate γ_i , and $\{A, B\}$ stands here for the anti-commutator $AB + BA$ of two matrices. The explicit form of matrices $\{L_i\}$ and of rates $\{\gamma_i\}$ depends on the specific problem at hand. In particular the physical properties of E are encoded in the rates $\{\gamma_i\}$.

C. Stochastic wave function: quantum dynamics as piecewise-deterministic processes

In Subsection I B, mixed quantum states have been introduced to account for classical-like stochasticity in the state vector, in addition to the purely quantum one. As a consequence, the density matrix (2) has been introduced together with its Markovian time evolution (5). The formalism in terms of density matrices describes the average response of a collection of identical quantum systems, the state vector of which has a certain amount of stochasticity. The density matrix can be regarded as an average of systems' state vectors, and its evolution (5) as the average time evolution of such an ensemble of quantum systems. One can however wonder whether it is possible to obtain a description of the evolution of a single element of this ensemble. In other words whether it is possible to write down, for a single quantum system, an equation for its state vector extending eq. (1) to the case of open system dynamics, in the same way as, for density matrices, eq. (5) extends (3) to the case of an ensemble of open systems. Since, as discussed in Subsection I B, the interaction with an environment generally "hides" part of the information about the state vector of a system S , its time evolution cannot be deterministic and must take into account the environmental-induced stochasticity. The two natural requirements for such a single-open-system dynamical equation is that it must reduce to the deterministic equation (1) for a closed system, and its average must reproduce eq. (5). This second requirement is fundamental if one wants the single-open-system equation to describe the dynamics of one element of the ensemble (2). There are many possible formulations of equations respecting these two requirements [9–16], the full treatment of which goes well beyond the scope of this introduction. Here we give a brief overview on what goes under the name of *Markovian stochastic wave-function approach* [9, 10, 14], which has the advantage of having a clear and direct experimental interpretation and has recently been employed to investigate quantum stochastic thermodynamics [17, 18].

Skipping the derivation (the details of which can be found in [9]) and with the same L_i, γ_i and \tilde{H}_S as in eq. (5), the equation for the evolution of the state vector $|\psi\rangle$ of an open quantum system can be given under the form of the stochastic differential equation

$$d|\psi\rangle = -\frac{i}{\hbar}\mathcal{L}(|\psi\rangle)dt + \sum_{i=1}^{N^2-1} \left(\frac{L_i|\psi\rangle}{|L_i|\psi\rangle|} - |\psi\rangle \right) dN_i, \quad (6)$$

where $|\cdot|$ is the norm in the Hilbert space. Eq. (6) is the sum of a deterministic time evolution with generator $\mathcal{L}(|\psi\rangle)$ and a stochastic contribution in terms of inhomogeneous Poisson processes $N_i = N_i(t)$ satisfying $dN_i dN_j = \delta_{ij} dN_i$ and

$$\mathbb{E}[dN_i(t)] = \gamma_i |L_i|\psi\rangle|^2 dt, \quad (7)$$

The generator of the deterministic evolution has the form

$$\mathcal{L}(|\psi\rangle) = \left(\tilde{H}_S - \hbar \frac{i}{2} \sum_{i=1}^{N^2-1} \gamma_i (L_i^\dagger L_i - |L_i|\psi\rangle|^2) \right) |\psi\rangle.$$

This deterministic evolution has the form of a (non-linear) Schrödinger equation, which can be shown for time-independent Hamiltonian \tilde{H}_S and Lindblad operators L_i to have the formal solution

$$|\psi(t)\rangle_{\text{Det}} = e^{-\frac{i}{\hbar} \hat{H} t} |\psi(0)\rangle, \quad (8)$$

through the effective non-Hermitian Hamiltonian $\hat{H} = \tilde{H}_S - \hbar \frac{i}{2} \sum_{i=1}^{N^2-1} \gamma_i L_i^\dagger L_i$. Note that, due to the non-Hermitian part $-\hbar \frac{i}{2} \sum_{i=1}^{N^2-1} \gamma_i L_i^\dagger L_i$, the norm of $|\psi(t)\rangle$ in eq. (8) generally decreases in time.

On the other hand, the stochastic contribution in (6) produces in the evolution of $|\psi(t)\rangle$ random instantaneous transitions. As evident from (6), there is a discrete and finite set of possible jumps for the state vector of the form

$$|\psi\rangle \rightarrow \frac{L_i|\psi\rangle}{|L_i|\psi\rangle|}, \quad i = 1, \dots, N^2 - 1. \quad (9)$$

Each of these jumps, due to property (7), happens at a rate $\gamma_i |L_i|\psi\rangle|^2 dt$: the dynamics of the state vector is thus a Markovian piecewise-deterministic process (PDP). It is possible to show that the waiting-time distribution during a deterministic evolution from the initial state $|\psi(0)\rangle$ is $f(t) = 1 - \|\psi(t)\rangle_{\text{Det}}\|^2$, which explains the meaning of a decreasing norm during deterministic evolutions. It is easy to see that eq. (6) reduces to the deterministic Schrödinger equation when $\gamma_i = 0 \forall i$ (closed-system case). It is also possible to show rigorously that

$$\mathbb{E}[|\psi(t)\rangle\langle\psi(t)|] = \rho(t), \quad (10)$$

$|\psi(t)\rangle$ being the solution of eq. (6), $\rho(t)$ the solution of eq. (5).

The above point proves that the trajectories given by eq. (6) are indeed a valid single-system representation of the ensemble dynamics. In addition, these trajectories have a direct and interesting experimental interpretation. To make this interpretation clear, it is convenient to state here that the Markovian master equation (5) is invariant under unitary or inhomogeneous transformations [9]. In the latter case the transformations $L_i \rightarrow L'_i$ and $\tilde{H}_S \rightarrow \tilde{H}'_S$ read

$$L'_i = L_i + \beta_i \mathbb{I}, \quad \text{and} \quad \tilde{H}'_S = \tilde{H}_S + \frac{1}{2i} \sum_{k=1}^{N^2-1} \gamma_k (\beta_k^* L_k - \beta_k L_k^\dagger) + \alpha \mathbb{I}, \quad (11)$$

where $\beta_i \in \mathbb{C}$ and $\alpha \in \mathbb{R}$. Despite leaving eq. (5) invariant, the transformation (11) changes eq. (6) while still assuring that $\mathbb{E}[|\psi(t)\rangle\langle\psi(t)|] = \rho(t)$. This means that different single-system-dynamics decompositions of the same ensemble dynamics are possible. It turns out that these different decompositions correspond to the different ways of performing continuous measurements on the environment E the system S is in contact with. Intuitively, since a direct measurement of S would collapse its state vector and thus stop its dynamics, one must follow the dynamics of system

S by indirect measures. Specifically, one looks for signatures, in the continuously-monitored state of E , of possible transitions happening in S . Thanks to the fact that E and S interact and that it is properly this interaction that causes departures from the closed-system dynamics, monitoring S through E is enough to reconstruct its dynamics. Under this interpretation, the deterministic parts of the evolution of S correspond to the absence of detected transitions in the state of E , while jumps correspond to the detection of a particular transition i .

D. Estimation for piecewise-deterministic processes

As explained above, the pure quantum state of an open system evolves as a piecewise-deterministic Markov process. In recent years, the literature has extensively investigated this class of stochastic processes, in particular for statistical purposes in a general setting [19, 20] or in the context of particular applications: while not exhaustive, applications considered are various, from cell cycle modeling [21, 22] to fatigue crack propagation analysis [23] through insurance risk models [24], food contaminants exposure [25], and neurobiology [26]. Nevertheless, to the best of our knowledge, no paper deals with statistical estimation in the particular context of quantum dynamics, whose specificities need to be taken into account. We think that three of them are particularly significant. First, the state space of quantum trajectories is the unit ball of a complex Hilbert space, which is a bit unusual. In addition, post-jump locations lie on the boundary so that the transition kernel does not admit a density with respect to the Lebesgue measure on the whole state space but only on the unit circle. For instance, the techniques developed by [27] for estimating the transition distribution do not apply in this context. Last but not least, the direct observation of the trajectory is problematic due to the wave-function collapse phenomenon, and can at most be performed only once at a specific time managed by the experimenter, while usual observation schemes assume repeated observations of the trajectory, either at the jump times or on a regular temporal grid.

II. PROBLEM FORMULATION

Let us imagine to have n_s copies of a quantum system S , each in contact with the same Markovian environment E . Assume that we know some properties of S (in particular, we know its Hamiltonian), but we do not know its initial state $|\psi(0)\rangle$. Also, we do not know the state of E , which is assumed not to evolve in time compatibly with the Born-Markov approximation. We assume to be allowed here to continuously monitor E , such that the trajectory of each single quantum system can be followed.

We wonder whether information on additional properties of S , on the initial state of its n_s copies and on the state of E can be inferred by looking at the system's trajectories. On top of the piecewise-deterministic trajectories, we allow a single direct measurement to be performed on each copy of S . This instantaneously stops the dynamics of S and hence destroys its trajectory, which means that after each such measurement a new copy of S must be considered and followed in time.

A. Atom-field interaction

We consider in particular our system S to be an atom² with two distinct energy levels only, a situation often encountered in practical applications in the fields of quantum information and quantum computation [28]. Be $|0\rangle$ and $|1\rangle$ these two energy levels, and be $\varepsilon_g = \varepsilon_1 - \varepsilon_0 > 0$ their energy gap. The system's Hamiltonian, expressed in the $\{|0\rangle, |1\rangle\}$ basis, simply reads

$$H_S = \begin{pmatrix} 0 & 0 \\ 0 & \varepsilon_g \end{pmatrix},$$

while most general expression for the system's state vector is

$$|\psi\rangle = c_0|0\rangle + c_1|1\rangle, \quad (12)$$

with $c_0, c_1 \in \mathbb{C}$ and $|c_0|^2 + |c_1|^2 = 1$. The (Markovian) environment E considered here is a thermal electromagnetic field, at the unknown temperature T . In a semi-classical treatment of the problem [29], in which S is considered a quantum system but E is treated classically, and in the weak-coupling limit, the atom interacts with the field through the dipole moment of its $|0\rangle \leftrightarrow |1\rangle$ transition. Such an interaction leads to either the absorption of a photon of energy ε_g from E (transition $|0\rangle \rightarrow |1\rangle$) or to the emission of an excitation of energy ε_g into E (transition $|1\rangle \rightarrow |0\rangle$). The atomic dynamics is given, on an ensemble level, by the master equation

$$\begin{aligned} \frac{d\rho}{dt} = & -\frac{i}{\hbar}[H_S, \rho] \\ & + \gamma_1(\sigma^- \rho \sigma^+ - \frac{1}{2}\{\sigma^+ \sigma^-, \rho\}) + \gamma_2(\sigma^+ \rho \sigma^- - \frac{1}{2}\{\sigma^- \sigma^+, \rho\}), \end{aligned} \quad (13)$$

which is of the form (5) with $L_1 = \sigma^- = |0\rangle\langle 1|$ describing the emission of a photon to E , $L_2 = \sigma^+ = (\sigma^-)^\dagger = |1\rangle\langle 0|$ the absorption of a photon from E with rates, respectively, $\gamma_1 = (1 + n(\varepsilon_g, T))\gamma_0$ and $\gamma_2 = n(\varepsilon_g, T)\gamma_0$. Here γ_0 is the atomic vacuum spontaneous emission rate and

$$n(\varepsilon, T) = \frac{1}{-1 + e^{\varepsilon/k_B T}} \quad (14)$$

is the average number of photons of energy ε in a field at temperature T , $k_B \simeq 1.38 \times 10^{-23} \text{ J K}^{-1}$ being Boltzmann's constant.

It is possible to solve eq. (13) analytically, obtaining

$$\rho(t) = \begin{pmatrix} p_0(t) & K(t) \\ K^*(t) & 1 - p_0(t) \end{pmatrix},$$

with

$$\begin{aligned} p_0(t) &= p_0(0)e^{-(\gamma_1+\gamma_2)t} + \frac{\gamma_1}{\gamma_1 + \gamma_2} (1 - e^{-(\gamma_1+\gamma_2)t}), \\ K(t) &= K(0)e^{\frac{i\varepsilon_g t}{\hbar}} e^{-\frac{\gamma_1+\gamma_2}{2}t} \end{aligned} \quad (15)$$

being, respectively, the $|0\rangle$ -state ensemble population and the so-called quantum coherence between states $|0\rangle$ and $|1\rangle$.

² By ‘‘atom’’ we mean here any quantum system whose internal structure we can model as having a discrete set of energy levels. Examples are real atoms, quantum dots, superconducting qubits, polarisation states of photons etc...

B. Piecewise-deterministic trajectories

On the other hand, when continuously monitoring the field, the dynamics of S can be followed under the form of a piecewise-deterministic process (PDP). In the specific example at hand, as a particular case of the general setting discussed in Subsection IC, more than one possibility exists for monitoring the field. Here we consider two possible schemes, equivalent respectively to the so-called *direct photodetection* and the so-called *homodyne photodetection* [9, 12]. In the first case the jump operators are simply σ^- and σ^+ with associated rates γ_1 and γ_2 respectively, the same as in eq. (13). This configuration corresponds to directly probing the field for photons emitted/absorbed by the atom. In the second case, four jump operators are introduced as $L_e^\pm = \sigma^- \pm i\beta$ and $L_a^\pm = \sigma^+ \pm i\beta^* = (L_e^\mp)^\dagger$ ($\beta \in \mathbb{C}$), with rates $\gamma_e^\pm = \frac{\gamma_1}{2}$ and $\gamma_a^\pm = \frac{\gamma_2}{2}$. This is a transformation of the kind (11) (it is easy to see that it does not change the Hamiltonian of the system) and, as such, produces a valid set of Lindblad operators. These operators correspond to monitoring the field E after it interferes with another local electromagnetic field of amplitude β , which is not directly coupled to S .

Note that the “direct-photodetection-like” scheme is obtained from the “homodyne-photodetection-like” scheme in the limit $\beta \rightarrow 0$. We will hence hereafter focus on the homodyne strategy alone. The deterministic part of the system’s trajectories is governed by the non-Hermitian Hamiltonian

$$\hat{H} = \begin{pmatrix} -\hbar\frac{i}{2}[\gamma_1|\beta|^2 + \gamma_2(1 + |\beta|^2)] & 0 \\ 0 & \varepsilon_g - \hbar\frac{i}{2}[\gamma_2|\beta|^2 + \gamma_1(1 + |\beta|^2)] \end{pmatrix} \quad (16)$$

while, using eqs. (9) and (12), the four possible jumps are

$$J_e^\pm : c_0|0\rangle + c_1|1\rangle \rightarrow \frac{1}{\sqrt{N_e^\pm}} \left((c_1 \pm i\beta c_0)|0\rangle \pm i\beta c_1|1\rangle \right), \quad (17)$$

$$J_a^\pm : c_0|0\rangle + c_1|1\rangle \rightarrow \frac{1}{\sqrt{N_a^\pm}} \left(\pm i\beta^* c_0|0\rangle + (c_0 \pm i\beta^* c_1)|1\rangle \right), \quad (18)$$

where N_e^\pm and N_a^\pm are normalization factors. Following eq. (7) the associated probabilities are

$$p_{e,a}^\pm = \frac{\gamma_{e,a}^\pm N_{e,a}^\pm}{\gamma_e^+ N_e^+ + \gamma_e^- N_e^- + \gamma_a^+ N_a^+ + \gamma_a^- N_a^-}. \quad (19)$$

Finally, given that the last jump has brought the system to the state $h_0|0\rangle + h_1|1\rangle$, the waiting-time distribution for the next jump is

$$f(\tau) = 1 - |h_0|^2 e^{-\tau[\gamma_1|\beta|^2 + \gamma_2(1 + |\beta|^2)]} - |h_1|^2 e^{-\tau[\gamma_2|\beta|^2 + \gamma_1(1 + |\beta|^2)]}. \quad (20)$$

C. Measures

As discussed in Subsection IC, a quantum trajectory (or PDP), is generated when the environment of an open quantum system is continuously monitored. This allows, in principle, to detect the transitions induced by the system-environment interaction and to determine whether the system has “jumped” to a new quantum state.

On top of that, we assume here that the analyst is allowed, only once per repetition of the PDP, to directly measure the quantum system. By virtue of Postulate 4 of Subsection IA, this radically interferes with the system’s dynamics and projects the state vector onto one eigenvector of the measured observable. This is the reason why only one direct measurement is allowed during the

PDP: after measuring, the PDP is fundamentally altered and no further information on the system's original dynamics can be extracted. Measuring properties of a single-system's wave function is a challenging but possible task [30, 31]. The quantity we choose to measure is, for the i -th trajectory in the state $|\psi_i(t_i)\rangle$ at time t_i ,

$$Y_{t_i}^i = |\langle 0|\psi_i(t_i)\rangle|^2, \quad (21)$$

i.e., the amplitude of the projection of the state onto the atomic ground state. Note that, in light of eq. (10),

$$\begin{aligned} \mathbb{E}[Y_{t_i}^i] &= \mathbb{E}[\langle 0|\psi_i(t_i)\rangle\langle\psi_i(t_i)|0\rangle] = \langle 0| \mathbb{E} [|\psi_i(t_i)\rangle\langle\psi_i(t_i)|] |0\rangle \\ &= \langle 0| \rho(t_i) |0\rangle = p_0(t_i). \end{aligned} \quad (22)$$

A specific example of distribution of the outcomes $Y_{t_i}^i$ on 10^2 repetitions of the atomic PDP is shown in the upper panel of Fig. 1. The bottom panel of Fig. 1 shows the r.h.s. (crosses) and the l.h.s. (solid line) of eq. (22).

III. ESTIMATION PROCEDURE

A. Strategy

We are interested in the estimation of the unknown parameters of the system, namely the initial condition $p_0(0)$ and the parameters γ_1 and γ_2 . As aforementioned, we observe a dataset composed of independent measures $Y_{t_i}^i$, $1 \leq i \leq n$, where the time of measurement t_i can be chosen by the analyst. In this chapter, we propose to apply an ordinary least squares estimation method that only takes advantage of the average behaviour of the measures expressed in eq. (22). Precisely, the estimator $(\hat{p}_0(0), \hat{\gamma}_1, \hat{\gamma}_2)$ is expected to be obtained by minimizing the function

$$V(p_0(0), \gamma_1, \gamma_2) = \sum_{i=1}^n (Y_{t_i}^i - p_0(t_i))^2,$$

where the dependency of p_0 on the three parameters is implicit. The expression of p_0 being rather complex, and in order to avoid gradient algorithms for minimizing the sum of squares function, we exploit the fact that the experimenter can manage the times of measurement to simplify the equations. First, as t goes to infinity,

$$p_0(t) \rightarrow \frac{\gamma_1}{\gamma_1 + \gamma_2}.$$

In addition, as t goes to 0, we have

$$p_0(t) \sim p_0(0) + t[\gamma_1 - p_0(0)(\gamma_1 + \gamma_2)].$$

Consequently, if the $n/2$ first measurements have been made in long time while the $n/2$ last measurements have been made in short time, the parameters can be estimated by simultaneously minimizing the approximated functions

$$V^l(\gamma_1, \gamma_2) = \sum_{i \leq n/2} \left(Y_{t_i}^i - \frac{\gamma_1}{\gamma_1 + \gamma_2} \right)^2, \quad (23)$$

$$V^s(p_0(0), \gamma_1, \gamma_2) = \sum_{i > n/2} (Y_{t_i}^i - p_0(0) - t_i[\gamma_1 - p_0(0)(\gamma_1 + \gamma_2)])^2, \quad (24)$$

where V^l does not depend on the initial value $p_0(0)$.

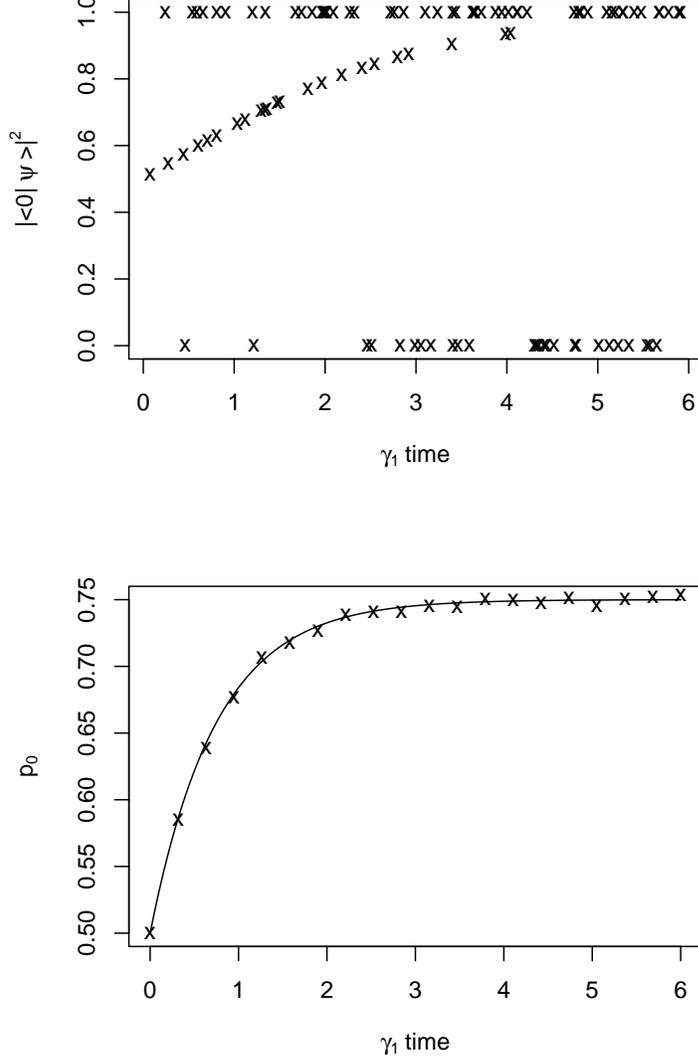


FIG. 1: Top: Distribution of measurement outcomes $Y_{t_i}^i$ (eq. (21)) on 10^2 trajectories, all having the same initial state $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ and measured at randomly-chosen timepoints t_i . Bottom: average value (22). Each point at time t_x corresponds to the average of $|\langle 0 | \psi_i(t_x) \rangle|^2$ over 10^4 trajectories, all having the same initial state $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$. The solid line is the analytical solution (15) of the ensemble dynamics. Other system parameters are $\varepsilon_g = 10^{14} \text{ rad} \cdot \text{s}^{-1}$ and $\beta = 0$.

B. Least-square estimators

It should be noticed that (23) and (24) can be easily expressed in terms of $p_0(0)$ and

$$u_1 = \frac{\gamma_1}{\gamma_1 + \gamma_2}, \quad (25)$$

$$u_2 = \gamma_1 - p_0(0)(\gamma_1 + \gamma_2). \quad (26)$$

With this reparametrization, we have

$$V^l(u_1) = \sum_{i \leq n/2} (Y_{t_i}^i - u_1)^2,$$

$$V^s(p_0(0), u_2) = \sum_{i > n/2} (Y_{t_i}^i - p_0(0) - t_i u_2)^2.$$

The main advantage for these new equations is that the three variables have been decoupled from each other. It is obvious to see that \hat{u}_1 defined as the average value of the $Y_{t_i}^i$ in long time, i.e.,

$$\hat{u}_1 = \frac{2}{n} \sum_{i \leq n/2} Y_{t_i}^i,$$

minimizes V^l . In addition, $V^s(p_0(0), u_2)$ is the cost function associated with classical linear regression, with $p_0(0)$ as the intercept and u_2 as the slope. The well-known solution of this minimization problem is expressed in terms of empirical mean, variance and covariance of the measures in short time,

$$\hat{u}_2 = \frac{\sum_{i > n/2} \left(t_i - \frac{2}{n} \sum_{i > n/2} t_i \right) \left(Y_{t_i}^i - \frac{2}{n} \sum_{i > n/2} Y_{t_i}^i \right)}{\sum_{i > n/2} \left(t_i - \frac{2}{n} \sum_{i > n/2} t_i \right)^2},$$

$$\hat{p}_0(0) = \frac{2}{n} \sum_{i > n/2} Y_{t_i}^i - \hat{u}_2 t_i. \quad (27)$$

The reparametrization (25) and (26) can be inverted and we get the following estimators of γ_1 and γ_2 ,

$$\hat{\gamma}_1 = \frac{\hat{u}_1 \hat{u}_2}{\hat{u}_1 - \hat{p}_0(0)}, \quad (28)$$

$$\hat{\gamma}_2 = \frac{(1 - \hat{u}_1) \hat{u}_2}{\hat{u}_1 - \hat{p}_0(0)}. \quad (29)$$

C. Numerical experiments

To test the performance of the estimators (27), (28) and (29) we performed several numerical experiments, by simulating sets of n trajectories according to eqs. (16) and (20), having chosen the atomic transition energy $\varepsilon_g = 10^{14} \text{ rad} \cdot \text{s}^{-1}$, a value falling into the infrared spectrum, following the high interest arising nowadays on technologies based on infrared quantum dots [32]. The initial state of each trajectory is $|\psi_{\text{init}}\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ and we fixed $\gamma_1 = 0.3 \text{ s}^{-1}$, $\gamma_2 = 0.1 \text{ s}^{-1}$.

As a first set of numerical experiments, we fixed the value $\beta = 0$, thus limiting ourselves to the case of direct photodetection, and simulated four groups of 10^2 sets of n trajectories, with $n = 50, 100, 500, 1000$. For each set of n trajectories, the procedure of Subsections IIC and IIIB was applied to produce the estimation of the three parameters $p_0(0)$, γ_1 and γ_2 . Fig. 2 shows the distribution of the 10^2 estimator values for each value of n (top: $p_0(0)$; middle: γ_1 ; bottom: γ_2). As clearly seen, the performance of the estimators (27), (28) and (29) increases significantly with

increasing n . The average value of each estimator is in very good agreement with the real value of the corresponding parameter (horizontal blue line in each panel).

As a second set of experiments, we investigated if and how different strategies for environmental measurements have an impact on the estimator performances. In particular, in the set of simulations shown in Fig. 3, we fixed the number of trajectories for each estimation to $n = 10^3$ and tuned the value of $\beta \in \mathbb{R}$ in the range $[0, 3]$. For each β -value, 10^2 groups of 10^3 trajectories were simulated, and estimators were calculated for each group. The boxplot distributions shown in the three uppermost panels of Fig. 3, for respectively $p_0(0)$, γ_1 and γ_2 , highlight the fact that the performance of the estimators does not seem to depend on the chosen measuring strategy. This in spite of the fact that the structure of the simulated trajectories strongly depends on such strategy, as shown in the bottom panel of Fig. 3 giving, for each simulated value of β , the average number of jumps in the corresponding set of trajectories, which increases quadratically with $|\beta|$.

IV. PHYSICAL INTERPRETATION

The two parameters γ_1 and γ_2 , whose value is estimated through the procedure presented in Subsection III B, contain important information on physical properties of both the atom and the electromagnetic field. Their estimation can be thus used to access unknown physical properties of both systems. Recall that $\gamma_1 = (1 + n(\varepsilon_g, T))\gamma_0$ and $\gamma_2 = n(\varepsilon_g, T)\gamma_0$, with the average photon number $n(\varepsilon_g, T)$ given by eq. (14) and the atomic vacuum spontaneous emission rate

$$\gamma_0 = \frac{|\mathbf{d}|^2 \varepsilon_g^3}{3\hbar^4 \pi \epsilon_0 c^3}, \quad (30)$$

where $\epsilon_0 \simeq 8.85 \times 10^{-12} \text{ F m}^{-1}$ is the vacuum permittivity, $c \simeq 2.998 \times 10^8 \text{ m s}^{-1}$ is the speed of light in vacuum and \mathbf{d} is the dipole moment vector of the atomic transition. This means that, assuming the knowledge of the energy gap ε_g of the atomic transition, one has access to the temperature T of the electromagnetic field as

$$T = \frac{\varepsilon_g}{k_B \ln \frac{\gamma_1}{\gamma_2}}. \quad (31)$$

Estimating γ_1 and γ_2 through atomic trajectories means thus that one can use the atom to probe the field temperature or, in other words, that the atom can be used as a field thermometer.

In addition, atomic properties can also be inferred. In particular, using now eqs. (14), (30) and (31) together with the definition of γ_1 and γ_2 one obtains

$$|\mathbf{d}|^2 = (\gamma_1 - \gamma_2) \frac{3\hbar^4 \pi \epsilon_0 c^3}{\varepsilon_g^3}, \quad (32)$$

which allows to estimate the square norm of the atomic dipole through observations of the atomic PDP. This is exemplified in Fig. 4, showing the estimation of both T and $|\mathbf{d}|$ through the estimators for γ_1 and γ_2 .

For $\gamma_1 = 0.3 \text{ s}^{-1}$, $\gamma_2 = 0.1 \text{ s}^{-1}$ and $\varepsilon_g = 10^{14} \text{ rad} \cdot \text{s}^{-1}$ one obtains $|\mathbf{d}| \sim 2 \times 10^{-31} \text{ C} \cdot \text{m}$ and $T \sim 700 \text{ K}$, values which correspond to the blue horizontal lines in the panels of Fig. 4. The good agreement shown in Fig. 4 between the estimations and the real values of T and $|\mathbf{d}|$ shows that the procedure leading to the estimators (28) and (29) can indeed be used to probe unknown physical properties of both the atom and the electromagnetic field.

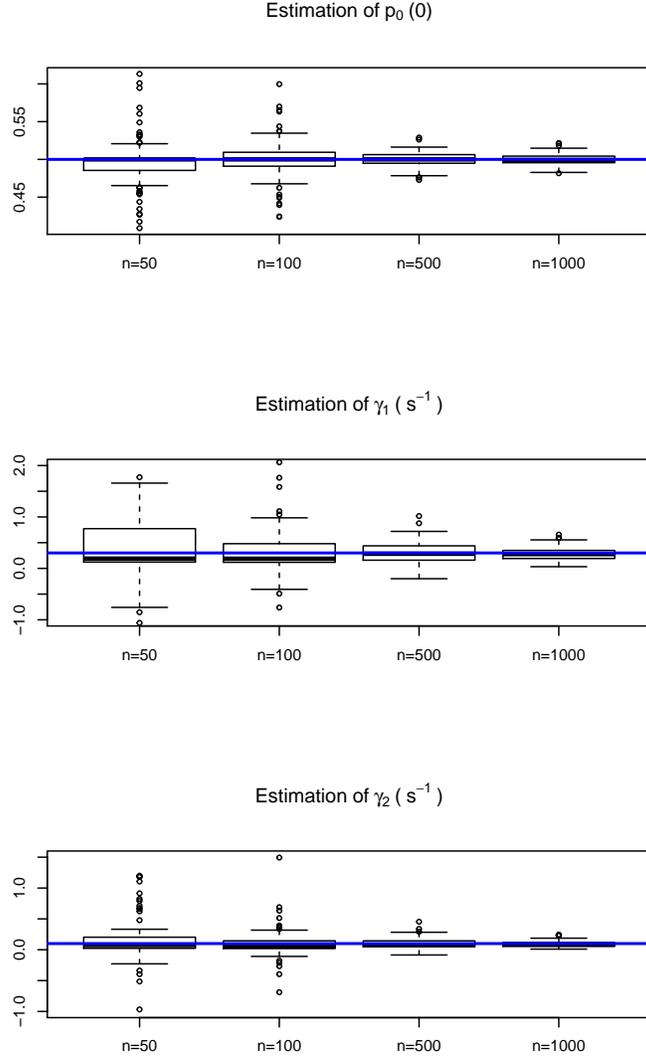


FIG. 2: Performance of estimators $\hat{p}_0(0)$ (eq. (27), top panel), $\hat{\gamma}_1$ (eq. (28), middle panel) and $\hat{\gamma}_2$ (eq. (29), bottom panel), against the number n of simulated trajectories. Each boxplot gives the distribution of estimator values over 100 repetitions of n trajectories. All trajectories have the same initial state all having the same initial state $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$. Blue horizontal lines in each panel give the actual parameter value ($p_0(0) = 0.5$, $\gamma_1 = 0.3$, $\gamma_2 = 0.1$). Other system parameters are $\varepsilon_g = 10^{14} \text{ rad} \cdot \text{s}^{-1}$ and $\beta = 0$.

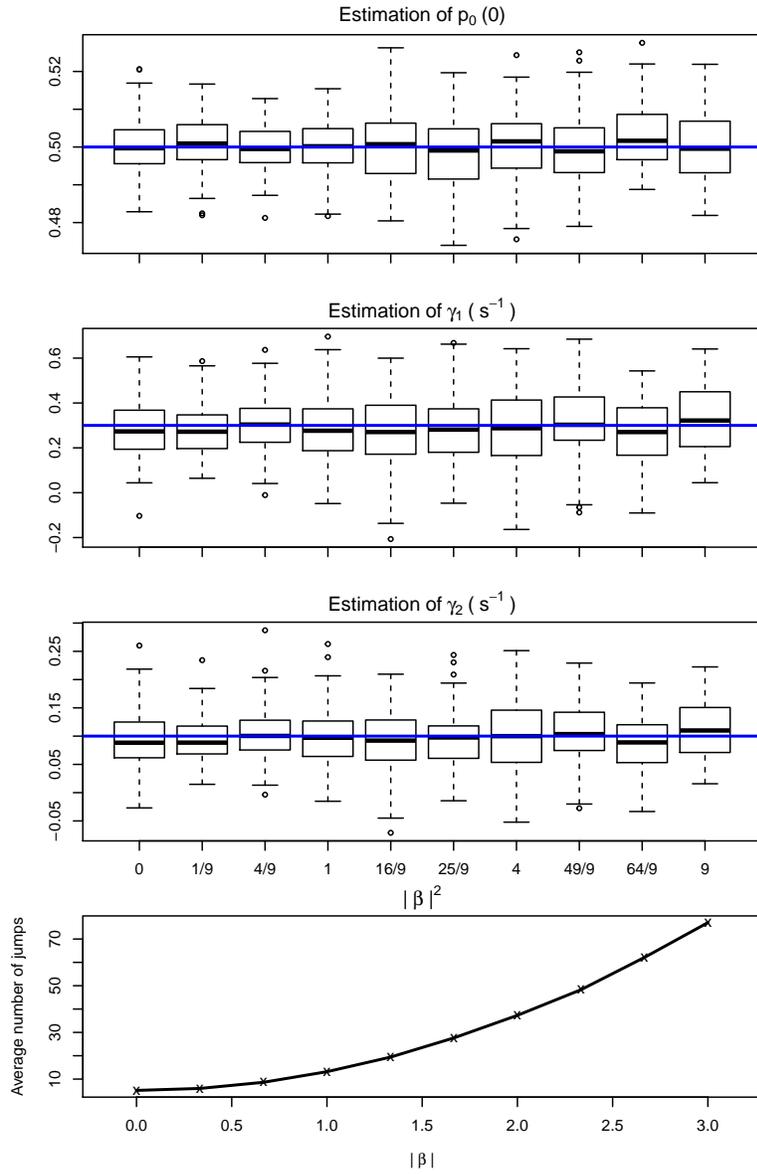


FIG. 3: Performance of estimators $\hat{p}_0(0)$ (eq. (27), top panel), $\hat{\gamma}_1$ (eq. (28), top-middle panel) and $\hat{\gamma}_2$ (eq. (29), bottom-middle panel), against variations of $|\beta|$, which has a major effect on the average number of jumps per trajectory (bottom panel). Each boxplot gives the distribution of estimator values over 100 repetitions of 10^3 trajectories, all having the same initial state $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$. Blue horizontal lines in each panel give the actual parameter value ($p_0(0) = 0.5$, $\gamma_1 = 0.3$, $\gamma_2 = 0.1$). The other system parameter is $\varepsilon_g = 10^{14} \text{ rad} \cdot \text{s}^{-1}$.

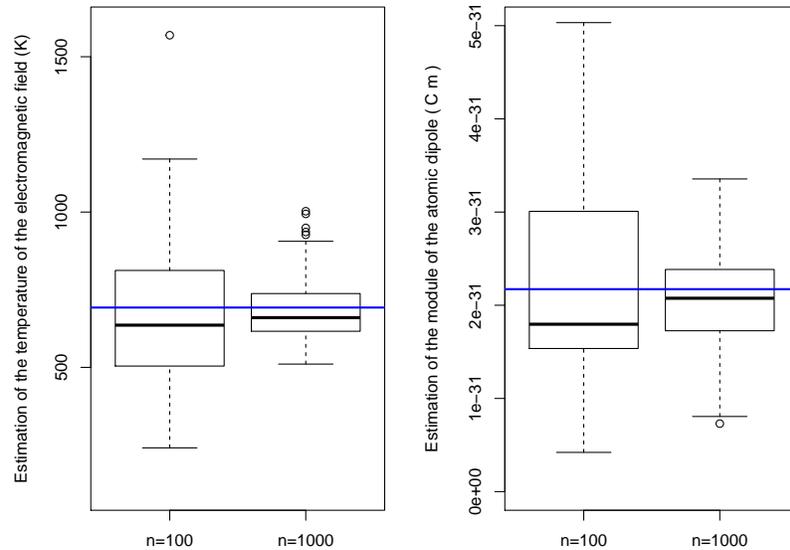


FIG. 4: Estimation of the environmental temperature T (eq. (31), left panel) and of the module of the atomic transition dipole (eq. (32), right panel) for 100 repetitions of either 10^2 or 10^3 trajectories, for the same parameter values as in Fig. 2. For comparison, the typical order of magnitude of the dipole moment of the hydrogen atom is 10^{-30} C · m.

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