NON-EQUILIBRIUM THERMODYNAMIC MODELING OF AN ATOM-FIELD STATE EVOLUTION WITH COMPARISONS TO PUBLISHED EXPERIMENTAL DATA

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ABSTRACT

The analysis of the decoherence phenomenon between the local states of an electromagnetic field mode and an atom, such as that experimentally studied in Cavity Quantum Electrodynamics (CQED), is presented in this paper. The equation of motion of Intrinsic Quantum Thermodynamics (IQT) is used to model the dynamics of the state of the general microscopic system constituted by the two distinguishable and indivisible elementary subsystems. The evolution of state of the composite, as well as the reduced states of its constituents, is traced from a state of non-equilibrium to a state of stable equilibrium. Results show how the entanglement and coherence initially present between the locally-perceived states of each subsystem are erased when the state of the composite system evolves towards a state of stable equilibrium. The results presented provide an alternative and comprehensive explanation to that obtained with the "open system" approach of Dissipative Quantum Dynamics (DQD) and its associated quantum master equations of the Kossakowski-Lindblad-Gorini-Sudarshan type. Results of the relaxation modeling are compared with those of decoherence obtained experimentally by the CQED group at Paris.

INTRODUCTION

Efforts of the scientific community to understand the fundamental behaviour of nature and as a consequence effectively develop new technologies has placed quantum entanglement and coherence in the spotlight. Understanding the loss of quantum entanglement and coherence is at the core of explaining the transition between the microscopic and macroscopic worlds [1, 2]. Furthermore, manipulation of these type of communication phenomena is of great importance for the development of nanometric devices such as, for example, quantum computers [3-5] and quantum cryptographic systems [6, 7].

Entanglement among zero-entropy states or coherence among non-zero-entropy states is produced when two initially independent systems interact with each other. During this interaction, their states become correlated and can no longer be described independently of each other, that is, a single nonseparable system behavior is observed for the states of the two constituents. According to unitary dynamics, the state of the newly born composite should evolve in a superposition of outcomes. Nevertheless, daily observations of Nature and experiments on microscopic systems [8, 9] indicate that a loss of coherence among the local states of the constituents is always present. For example, during the physical measurement of a nonseparable microscopic system (e.g., a particle), the macroscopic measuring device (meter) gets entangled with the state of the particle and there after behaves as a macroscopic system in a superposition of states. The particle-meter composite system is then created, and an understanding of the loss of correlations between its constituents is at the core of quantum mechanics. Different theories are proposed to describe this phenomenon. One of them, that of dissipative quantum dynamic (DQD), considers that after its first entanglement with the particle, the meter gets involved into a second entanglement, this time with its surrounding environment, which provokes a fast dissipation of its quantum coherence originating from its initial entanglement with the

atom [1, 2]. Spontaneous relaxation is then modeled under the concept of the so-called "open-system model", which assumes that the system interacts with a thermal bath of harmonic oscillators (reservoir). The loss of coherence, disentanglement, or spontaneous relaxation is attributed to an irreversible reduction process resulting from weak interactions between the system and reservoir. Under this assumption, the dissipation phenomenon results from a loss of information only. The dynamic equation of DQD is a linear Markovian quantum master equations (i.e., those of the Kossakowski-Lindblad-Gorini-Sudarshan type [10-12]). These type of equations mimic well the non-linear dissipative behavior of simple systems. However, a proper description of the non-linear dynamics of the state of composite systems is not achieved [13, 14].

In this paper, the modeling of the non-linear dynamic behavior of the state of a composite system formed by an atom and an electromagnetic field mode is developed using IQT and its dynamical law of time evolution along the direction of steepest entropy ascent (SEA), which is an effective implementation of the locally maximal entropy production (LMEP) principle [15-17]. The state of the composite (closed and adiabatic) microscopic system evolves in time towards stable equilibrium, resulting in the loss of correlations between its constituents. The non-linear IQT equation of motion consists of two terms, the first of which captures the unitary, Hamiltonian dynamics of the Schrödinger-von Neumann equation, and the second the non-linear dynamics of a dissipative evolution in state based on the principle of SEA [16-19], which allows each constituent to follow the path of locallyperceived SEA [20]. Within the IQT framework, the dissipative aspects of the time evolution emerge from the non-Hamiltonian terms in the IOT equation of motion. Thus, instead of focusing on the non-Hamiltonian effects of the interactions between a microscopic system and its surroundings, the IQT description assumes the composite system to be isolated and its time evolution to be intrinsically non-Hamiltonian. In so doing, a loss of quantum entanglement or coherence is fully predicted.



Figure 1. Schematic representation of an atom-field Cavity QED experiment [21].

CQED EXPERIMENTAL TECHNIQUE BY THE GROUP AT PARIS

The description of the experiments as well as the values used in the present modeling are based on the work developed by the CQED group of Haroche and co-workers at Paris [9, 21-26]. The reader is encouraged to visit these references for a thorough description of the theoretical background, experimental setup, and measurements developed on decoherence between the local states of the atom and the electromagnetic field mode. The description provided in the rest of this section is according to our understanding of these experiments.

А schematic representation of the experimental configuration is depicted in Figure 1. Rubidium atoms are contained in an oven B from which one atom in state $|\psi_{R}\rangle = |e\rangle$ (excited level) is selected and subsequently subjected to a classical resonant microwave $\pi/2$ pulse in R₁ supplied by the source S'. This creates a state in a superposition of circular Rydberg levels $|e\rangle$ and $|g\rangle$ (ground level) for the atom, corresponding to principal quantum numbers 51 and 50, respectively. Afterwards, the atom is allowed to enter the high-Q quantum cavity C that contains an electromagnetic field mode in a Fock state $|\alpha\rangle$ previously injected into the cavity by an external source S. The atom and cavity are off-resonant, thereby, absorption of photons is not exhibited during the interaction, and the atom shifts only the phase of the field mode by an amount ϕ . This dephasing provokes the coupling of the excited level of the atom to the field mode state with phase $|\alpha e^{i\phi}\rangle$ ($|\alpha_0\rangle$) and the coupling of the ground state of the atom to the field mode state with phase $|\alpha e^{-i\psi}\rangle$ ($|\alpha_1\rangle$). In this manner, an entanglement between the states of the constituents is created such that

$$\left|\psi_{C}\right\rangle = \frac{1}{\sqrt{2}}\left(\left|e,\alpha_{0}\right\rangle + \left|g,\alpha_{1}\right\rangle\right) \tag{1}$$

After leaving the cavity, the atom is subjected again to a resonant microwave pulse in R_2 equal to that at R_1 , mixing the atom energy levels and creating a "*blurred*" state for the composite, which preserves the quantum ambiguity of the field phase such that

$$\left|\psi_{R_{2}}\right\rangle = \frac{1}{2}e^{-i\phi}\left|e\right\rangle\left(\left|\alpha_{0}\right\rangle - \left|\alpha_{1}\right\rangle\right) + \frac{1}{2}\left|g\right\rangle\left(\left|\alpha_{0}\right\rangle + \left|\alpha_{1}\right\rangle\right)$$
(2)

Finally, the excited level state of the Rb atom is observed and recorded by a detector D.

In order to measure the decay of coherence left on the field mode state by the atom, a second atom of identical characteristics of that of the first one is put through the same path after a delay time t_d . The reading of the state of the second atom at D uncovers the effects left by the first atom on the state of the field mode.

A theoretical description of the experimental observations is provided by [23] in the form the following correlation signal:

$$\eta(t_d) = \frac{1}{2} e^{-2n\left(1 - e^{-\gamma t_d}\right) \sin^2 \phi} \cos\left[n\left(1 - e^{-\gamma t_d}\right) \sin 2\phi\right]$$
(3)

where n = 3.3 is the average number of photons in the field mode, $\gamma = 1/T_R$, and T_R is the photon lifetime.

MODEL DESCRIPTION

Atom-field Jaynes-Cummings Hamiltonian

In the modeling of a field mode-atom system, it is common that the single mode of an electromagnetic field is assumed to be quantized and treated as a two-level-type harmonic oscillator fully represented in subspace \mathcal{H}_F , while the atom is treated as a two-level-type spin- $\frac{1}{2}$ particle fully represented in subspace \mathcal{H}_A [27-29]. This represents the simplest model in which light and matter can interact.

The Hamiltonian on $\mathscr{H} = \mathscr{H}_A \otimes \mathscr{H}_F$ describing the total energy of the composite is the traditional Jaynes-Cummings Hamiltonian [30-32] (in the rotating-wave approximation)

$$H = H_0 + V \tag{4}$$

where

$$H_0 = \frac{1}{2}\hbar\omega_a \left(\sigma^z \otimes I_F \right) + \hbar\omega_f \left(I_A \otimes N \right)$$
⁽⁵⁾

$$V = \frac{1}{2}\hbar\Omega_0 \left(a \otimes \sigma_+ + a^{\dagger} \otimes \sigma_- \right)$$
(6)

Here \hbar is the reduced Planck constant, σ^z is the *z*-Pauli operator, σ_+ and σ_- are the raising and lowering ("spin-flip") operators, a^{\dagger} and a are the creation and annihilation operators, and $N = a^{\dagger}a$ is the photon number operator. ω_a is the transition frequency between the excited and ground energy levels of the atom, ω_f is the cavity frequency, and Ω_0 the Rabi frequency which indicates the strength of the atom-field interaction.

For the present model, values taken from [9] are used. The transition frequency between the excited and ground energy levels of the atom is $\omega_a/2\pi = 51.099 \text{ GHz}$, the Rabi frequency is $\Omega/2\pi = 24 \text{ kHz}$, and a detuning $\delta/2\pi = 70 \text{ kHz}$ ($\delta = \omega_a - \omega_f$) is provided.

IQT state evolution dynamics

The generators of the motion for the isolated atom-field mode composite system is given by the set $R = \{I, H\}$ with the identity operator I expressed as $I = I_A \otimes I_F$ and the Hamiltonian operator by Eq. (4). The IQT equation of motion is [20]

$$\frac{d\rho}{dt} = -\frac{i}{\hbar} [H, \rho] - \left(\frac{1}{\tau_A} D_A \otimes \rho_F + \frac{1}{\tau_F} \rho_A \otimes D_F\right)$$
(7)

where the first term on the right-hand side describes the unitary Hamiltonian dynamics of the system and the second the non-Hamiltonian dissipation dynamics. The operator $[H, \rho] = H\rho - \rho H$ is the commutator between the Hamiltonian and the density or state operator, $\rho_A \equiv \text{Tr}_F \rho$ and $\rho_F \equiv \text{Tr}_A \rho$ are the reduced state operators, and τ_A and τ_F are time functionals or scalars that are a particular characteristic of each subsystem. For the case presented, they are assumed to be constants.

A correlation functional or entropy of entanglement function is [20]

$$\sigma_{AF}(\rho) = \operatorname{Tr}(\rho \ln \rho) - \operatorname{Tr}_{A}(\rho_{A} \ln \rho_{A}) - \operatorname{Tr}_{F}(\rho_{F} \ln \rho_{F})$$
(8)

It measures the coherence between the constituents of the system. The norm of the commutator operator $(C = i[H, \rho])$ is

$$\left\|C\right\| = \operatorname{Tr}\left(CC^{\dagger}\right) \tag{9}$$

and is used as an indicator of how the off-diagonal elements of the matrix representing the state operator evolve towards zero. It can, thus, also be thought of as a measure of the evolution of the coherence of the constituents.

The rate of change of the correlation functional given by Eq. (8) is expressed as

$$\frac{d(\sigma_{AF}(\rho))}{dt} = \dot{\sigma}_{AF}\big|_{H} - \dot{\sigma}_{AF}\big|_{D}$$
(10)

where the first term on the right-hand side represents the contribution, which the Hamiltonian term of Eq. (7) makes to the rate of change of the correlation functional. The second term on the right-hand side represents the contribution of the dissipative term of Eq. (7). Based on the characteristics of Eq. (7), it is has been conjectured [20] that $\dot{\sigma}_{AF} \mid_D$ only destroys correlations between the constituents, namely, it should be nonnegative at all times.

Important ingredients of the IQT model are the local observables given by the linear local operators

$$(H)^{A} \equiv \operatorname{Tr}_{F}\left[\left(I_{A} \otimes \rho_{F}\right)H\right]$$
(11a)

$$(H)^{F} \equiv \operatorname{Tr}_{A}\left[\left(\rho_{A} \otimes I_{F}\right)H\right]$$
(11b)

which represent the local effective reduced Hamiltonians and can be interpreted as the *"locally perceived energy"* of the overall system by each constituent [16, 20], and the local observables given by the nonlinear local operators

$$(S)^{A} \equiv -k_{B} \operatorname{Tr}_{F} \left[(I_{A} \otimes \rho_{F}) B \ln \rho \right]$$
(12a)

$$(S)^{F} \equiv -k_{B} \operatorname{Tr}_{A} [(\rho_{A} \otimes I_{F}) B \ln \rho]$$
(12b)

which represent the local effective reduced entropy operators and can be interpreted as the "*locally perceived entropy*" of the overall system by each constituent [16, 20].

The entropy of the overall isolated, composite, microscopic system is given by the von Neumann entropy relation [33]

$$S = -k_B \operatorname{Tr}(\rho \ln \rho) \tag{13}$$

where k_B is Boltzmann's constant.

For the IQT modeling, it is considered that t = 0 when the state of the atom is detected in its excited level state at D. The initial state operator

$$\boldsymbol{\rho}_{0} = \left| \boldsymbol{\psi}_{R_{2}} \right\rangle \left\langle \boldsymbol{\psi}_{R_{2}} \right| \tag{14}$$

for the composite represents a pure (zero entropy) state. In order for the state operator to evolve in time according to Eq. (7), a slight perturbation in agreement with [34] is induced. A value of $\lambda = 0.95$ is used in the perturbation in order to start the evolution in a very close state to the original zero-entropy initial state ($\lambda = 1$) given by Eq. (14). Values for $2\phi = 100^{\circ}$ [9] and the probability of the atom to be on its excited level state $P_e \approx 1$ are used.



Figure 2. Evolution of the norm ||C|| of the commutator term.



Figure 3. Entropy evolution corresponding to the composite system.



Figure 4. Energy-entropy diagram depicting the evolution in state of the composite system.

In the next section, the internal-relaxation time in the IQT equation of motion for each constituent is considered to be a real positive constant with values of $\tau_A = \tau_F = 300$ ms. This value is chosen because it is long enough to show well the various features of the state evolution in time of the composite system and its constituents. As seen below in the comparison with the experimental results of [9], a value of 0.26 ms is also used.

RESULTS

Figure 2 shows the norm of the commutator operator formed by the Hamiltonian and density operators, as given by Eq. (9). This shows how the off-diagonal elements in the overall density or state matrix are decaying with time as the system evolves towards a state of stable equilibrium. Thus, it is also an indicator on the degree to which the coherence between the constituents is being dissipated in time. As seen in the figure, the steepest descent occurs at the beginning of the time evolution. This steep descent is in accord with the steepestentropy-ascent principle pictorially described in Figure 3 for the entropy evolution. Note that only the first part of the complete evolution in state of the composite system is depicted in Figures 2 and 3, i.e., that part from the initial perturbed state A_0 in Figure 4 to state A_1 which occurs at $t/\tau = 5 \times 10^4$. Both states are non-equilibrium states quite far from that of stable equilibrium, i.e., state A_{se} . The latter is estimated to occur at or after $t/\tau = 5.2 \times 10^6$ based on the simulation actually completed, which was stopped at state A_2 after an elapsed time of $t/\tau = 6 \times 10^5$ (also a non-equilibrium state), since the state of the system at this point was evolving very slowly, i.e., asymptotically in a non-linear manner, towards A_{se} and the primary coherence and decoherence features of interest had already been captured.

Figure 5a depicts the evolution of the local density operator for the electromagnetic field mode. When the atom is detected in its excited level state, the state of the electromagnetic field is projected into a state of maximum local coherence. Subsequently, this local coherence decays in a steep fashion according with the evolution of Eq. (7). Figure 5b shows the evolution of the local density operator for the Rb atom where revival and death of its local coherence is observed during the evolution but with ever smaller amplitudes until the local coherence dies out at stable equilibrium.

Figure 6 shows the evolution of the rate of change of the contribution of the dissipation term of the equation of motion to the rate of change of the entropy correlation functional. Its value is non-negative always, showing that the dissipative term of the equation of motion does not create correlations between the constituents, but instead always destroys the correlations formed during the initial interaction between the constituents.



Figure 5. Evolution of the reduced density operators for (a) the electromagnetic field mode and (b) the Rb atom.



Figure 6. Rate of change $\sigma_{AF}|_D$ corresponding to the contribution of the dissipative term of Eq. (7) to the rate of change of the correlation functional or entropy of entanglement in Eq. (10).



Figure 7. Comparison of the loss of coherence predicted by IQT (green) and by the correlation function of [23] (blue) with the CQED experimental results of the group at Paris [9] (red triangles).

In Figure 7, the results of the present model are compared to experimental data reported in the literature by Haroche and coworkers [9]. The red triangles correspond to average values of experimental measurements obtained from [9]. The blue line corresponds to the theoretical prediction made using the correlation functional given by Eq. (3) [23]. The initial point of the correlation has been moved in accord with [9] from a value of 0.5 to 0.18 on the vertical axis to take into account experimental imperfections. The detection of the atom in the excited level state projects the state of the field in a maximally coherent local state. Thus, ||C|| can be used as a direct indicator of how the coherence of the electromagnetic field mode is being dissipated in time. The green line corresponds to $\|C\|$ using a value of $\tau_A = \tau_F = 0.26$ ms for the internal-relaxation times of the constituents in the equation of motion. This is comparable to the characteristic time reported for the CQED experiment in [35]. As in the case of the correlation functional, the maximum value for $\|C\|$ is moved to 0.18 in the vertical axis.

As can be seen in the figure, this decoherence indicator of IQT predicts the experimental data well, especially at the beginning and at the end of the decoherence evolution. A very slight deviation from the experimental values is observed with the fourth and fifth values but this is well within the error bars for the experiment indicated in the figure. Thus, this deviation may well correspond to normal imperfections in the experimental equipment such as the quality of reflexion of the mirrors, which allows a leak of photons from the cavity [25,

36]. Another factor may be that the value chosen for the internal-relaxation times τ_A and τ_F do not completely take into account the physical characteristics of the constituents. For example, it may be that slightly differing values for each relaxation time are needed or that these times are instead functionals of the state operator as described in [15, 34]. Of course, this is still an open area of research.

CONCLUSIONS

In this paper, an approach based on the principle of steepest entropy ascent, which provides the basis for the non-linear IQT equation of motion, is applied to the case of a composite microscopic system consisting of an atom and an electromagnetic field mode, the simplest model in which matter and light can be examined. Results show how the coherence of the composite system is dissipated when the system evolves towards a state of stable equilibrium and how this affects the local coherence of each constituent. For the electromagnetic field mode, the local coherence decays from some maximum to zero. The loss of coherence of the electromagnetic field follows the same trend as for the composite system. For the atom, the coherence is zero at the beginning of the evolution. Subsequently, however, several revivals and deaths of the coherence for the atom are observed. Nevertheless, even the amplitudes of these revivals and deaths decay with time.

Finally, the decoherence phenomenon predicted with the IQT model is compared to the experimental data of Haroche and co-workers [9]. The comparison shows that IQT prediction is in good agreement with the experiments and is, in fact, in much better agreement than that for the correlation function developed for this experiment in [23].

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