

Bath-induced correlations in an infinite-dimensional Hilbert space[★]

Marco Nizama^{1,a} and Manuel O. Cáceres^{2,b}

¹ Departamento de Física, Universidad Nacional del Comahue, 8300 Neuquén, Argentina

² Centro Atómico Bariloche, CNEA, Instituto Balseiro and CONICET, 8400 Bariloche, Argentina

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Abstract. Quantum correlations between two free spinless dissipative distinguishable particles (interacting with a thermal bath) are studied analytically using the quantum master equation and tools of quantum information. Bath-induced coherence and correlations in an *infinite-dimensional* Hilbert space are shown. We show that for temperature $T > 0$ the time-evolution of the reduced density matrix cannot be written as the direct product of two independent particles. We have found a time-scale that characterizes the time when the bath-induced coherence is maximum before being wiped out by dissipation (purity, relative entropy, spatial dispersion, and mirror correlations are studied). The Wigner function associated to the Wannier lattice (where the dissipative quantum walks move) is studied as an indirect measure of the induced correlations among particles. We have supported the quantum character of the correlations by analyzing the geometric quantum discord.

1 Introduction

In many practical situations where classical mechanics is enough to make a good description of a system, the interaction with a surrounding (bath) leads to dissipation and fluctuations. This program has also been extended to quantum mechanics concluding with fundamental results which can be summarized in the Fluctuation-Dissipation theorem, see [1,2] and references therein. Nevertheless, if we wish to describe the quantum non-equilibrium evolution the problem is inevitably outside of the scope of the previous Kubo-like approach. Other approximations must be introduced to work out an *open* quantum mechanics system [3]. Of importance is the analysis of the quantum mechanics correlations generated during the elapse of time of the interaction with a measurement apparatus [2]. In particular quantum mechanics correlations in a bipartite system have generated much interest for various tasks such as computing [4], imaging and metrology [5,6]. Thus, the understanding of the mechanism of decoherence is an issue of great interest as it would allow progress in construction of quantum mechanics devices [2].

The effect of a thermal quantum bath \mathcal{B} on a microscopic system \mathcal{S} has in particular been much discussed, the general consensus being that \mathcal{B} leads to dissipation

and decoherence on \mathcal{S} . Breaking the isolation of \mathcal{S} is then believed to significantly increase the decoherence [4,7,8]. Nevertheless, if this were true for all quantum mechanics open systems, no matter how small is the interaction with \mathcal{B} , fluctuation and dissipative effects would become very costly for the operation of quantum mechanics devices as needed in quantum computation. Indeed very recently it has been shown that entanglement between two qubits can be generated if the two qubits interact with a common thermal bath [9], also research on quantum information processing – in finite dimensional systems – have led to the picture of entanglement as a precious resource [10–13]. Additional studies concerning the analysis of a common bath vs individual baths have led to support the idea of bath-induced correlations in Markovian and non-Markovian approximations [14,15]. A related result has also been found where the role of non-Markovian effects for the quantum entanglement has been studied [16].

In this context an important point of view is achieved if we could analyze systems associated with an *infinite* dimensional Hilbert space. However, this is not a simple task for dissipative systems using the quantum information theory. In this work we propose to study – analytically – quantum correlations between two particles (in an infinite *discrete* dimensional Hilbert space) interacting with a thermal bath. Then we will show that indeed the bath \mathcal{B} generates not only dissipation, but induces coherence and correlations between particles immersed on it. In order to prove this fact, we will do exact calculations of the dynamics of spinless quantum walks [17–20]. Then exact analytic results for the induced correlations

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^a e-mail: marco.nizama@fain.uncoma.edu.ar

^b e-mail: caceres@cab.cnea.gov.ar

can be computed showing that \mathcal{B} may generate correlations between particles originally uncorrelated. In what follows, we present calculations to measure correlations and so to define a characteristic time-scale for a maximum coherence in the system before being wiped out by dissipation. We prove that these correlations are of quantum mechanics nature using the tools of quantum information theory, thus we show that our results can be used to measure the quantum to classical transition as we have already done studying associated qubit systems [21,22].

The simplest implementation that reflects the role of a coherent superposition can be proposed in the framework of quantum walk experiments, or its numerical simulations [23–27]. A Dissipative Quantum Walk (DQW) has also been defined as a spinless particle moving in a lattice and interacting with a phonon bath [17,18,20–22,28,29]. These models can also be extended considering a many-body description as we present here. In particular in this work we will implement explicit calculations for a system constituted by two distinguishable DQW's. Therefore, our approach can be used to tackle this general problem pointing out the interplay between dissipation and the bath-particle interaction.

A non-Markov extension of the present DQW model can also be introduced using the Continuous-Time Random Walk (CTRW) approach introduced by Montroll and Weiss [30,31]. In Appendix A a short review on the subject of quantum jumps in presented, this picture can also be related to the random quantum maps approach in the context of the Renewal theory [32].

2 Dissipative quantum walks

A model of two free distinguishable particles coupled to a common bath \mathcal{B} can be written using the Wannier base in the following way. Let the total Hamiltonian be $H_{\mathcal{T}} = H_{\mathcal{S}} + H_{\mathcal{B}} + H_{\mathcal{SB}}$, here $H_{\mathcal{S}}$ is the *free tight-binding* Hamiltonian [33] (our system \mathcal{S}), which can be written in the form:

$$H_{\mathcal{S}} = 2E_0\mathbf{I} - \frac{\Omega}{2} \left(a_{12}^{\dagger} + a_{12} \right),$$

here $\{a_{12}^{\dagger}, a_{12}\}$ are shift operators for the particles labeled 1 and 2, and \mathbf{I} is the identity in the Wannier base

$$\mathbf{I} = \sum_{s,s'} |s, s'\rangle \langle s, s'|, \quad (1)$$

then:

$$a_{12}^{\dagger} |s_j, s_l\rangle = |s_j + 1, s_l\rangle + |s_j, s_l + 1\rangle \quad (2)$$

$$a_{12} |s_j, s_l\rangle = |s_j - 1, s_l\rangle + |s_j, s_l - 1\rangle. \quad (3)$$

We note that a “shift operator” translates each particle individually. Here we have used a “pair-ordered” bra-ket $|s_j, s_l\rangle$ representing the particle “1” at site s_j and particle “2” at site s_l . From equations (2) and (3) it is simple to see that $[a_{12}^{\dagger}, a_{12}] = 0$ and the fact that

$$a_{12} a_{12}^{\dagger} |s_j, s_l\rangle = 2|s_j, s_l\rangle + |s_j - 1, s_l + 1\rangle + |s_j + 1, s_l - 1\rangle.$$

$H_{\mathcal{B}}$ is the phonon bath Hamiltonian $H_{\mathcal{B}} = \sum_n \hbar\omega_n \mathcal{B}_n^{\dagger} \mathcal{B}_n$,

thus $\{\mathcal{B}_n^{\dagger}, \mathcal{B}_n\}$ are bosonic operator characterizing the thermal bath at equilibrium.

The term $H_{\mathcal{SB}}$ in the total Hamiltonian represents the interaction term between \mathcal{S} and \mathcal{B} , here we use a linear interaction between the particles and the bath operators. Our model is a many-body generalization of the van Kampen approach used to address the nature of a physical dissipative particle interacting with a boson bath [18]. Because the shift operators $a_{1,2}$ and a_{12}^{\dagger} are constant of motions, any bath interaction with these shift operators will lead to a completely positive infinitesimal generator, see Kossakowski and Lindblad [3]. Thus, for two *distinguishable* particles we propose the interaction term $H_{\mathcal{SB}}$ in the form

$$H_{\mathcal{SB}} = \hbar\Gamma \left(a_{12} \otimes \sum_n v_n \mathcal{B}_n + a_{12}^{\dagger} \otimes \sum_n v_n^* \mathcal{B}_n^{\dagger} \right), \quad (4)$$

where v_n represents the spectral intensity weight function from the phonon bath at thermal equilibrium, and Γ is the interaction parameter in the model. We have chosen this interaction Hamiltonian in order to recover the classical master equation for two independent random walk in the case when $\Omega = 0$, for a more extended discussion on this issue see Appendix A in [21,31].

In order to study the non-equilibrium evolution of \mathcal{S} we derive from $H_{\mathcal{T}}$, eliminating the bath variables, a dissipative quantum infinitesimal generator (see Appendix A). Tracing out bath variables in the Ohmic approximation and assuming as initial state of the total system a density matrix in the form of a product

$$\rho_{\mathcal{T}}(0) = \rho(0) \otimes e^{-H_{\mathcal{B}}/k_B T} / Z,$$

where $Z = \text{Tr}(e^{-H_{\mathcal{B}}/k_B T})$, we can write the Markov Quantum Master Equation (QME) [2,3,20]:

$$\begin{aligned} \dot{\rho} = & \frac{-i}{\hbar} [H_{eff}, \rho] + \frac{D}{2} \left(2a_{12}\rho a_{12}^{\dagger} - a_{12}^{\dagger} a_{12} \rho - \rho a_{12} a_{12}^{\dagger} \right) \\ & + \frac{D}{2} \left(2a_{12}^{\dagger} \rho a_{12} - a_{12} a_{12}^{\dagger} \rho - \rho a_{12}^{\dagger} a_{12} \right), \end{aligned} \quad (5)$$

here $D \equiv \Gamma^2 k_B T / \hbar$, where T is the temperature of the bath \mathcal{B} . In the present paper we are interested in solving this QME with a localized initial condition in the Wannier lattice, i.e., $\rho(0) = |s_1, s_2\rangle \langle s_1, s_2|$.

Adding $-2E_0 + \Omega$ to $H_{\mathcal{T}}$ the effective Hamiltonian turns to be

$$H_{eff} = \Omega \left(\mathbf{I} - \frac{a_{12}^{\dagger} + a_{12}}{2} \right) - \hbar\omega_c a_{12} a_{12}^{\dagger}, \quad (6)$$

where $\omega_c \equiv 2\tilde{\omega}_c \Gamma^2$ is related to the frequency cut-off $\tilde{\omega}_c$ in the Ohmic approximation [3,18,20]. It can be seen from the *strength function* $g(\omega)$ of thermal oscillators (defined by $g(\omega) \Delta\omega \leftrightarrow [\sum_n v_n^2]_{\{\omega < \omega_n < \omega + \Delta\omega\}}$), that the high-frequency oscillators (beyond $\tilde{\omega}_c$) only modify the effective Hamiltonian, that is its unitary evolution, see Appendix A. This von Neumann dynamics can be defused

by going to the interaction representation. However, here we will be interested in studying the non-equilibrium evolution of the system as a function of the rate of energies Ω and $D \equiv \Gamma^2 k_B T / \hbar$. Then, in order to simplify the analysis of the QME (5) we will drop-out the term $\hbar\omega_c a_{12} a_{12}^\dagger$ in the effective Hamiltonian, which only produces additional reversible coherence. Under the assumption that $\hbar\tilde{\omega}_c/k_B T \ll 1$, the dissipative coefficient D appearing in (5) depends on the strength function and the thermal bath correlation function. This terms only involves oscillators in the low-frequency region. It is also possible to see that the Markov approximation used to get (5) involves a *coarse-grained* time scale such that $\tilde{\omega}_c \Delta t \gg 1$ in addition to a second order weak interaction approach, which at the end leads to the damping dissipative factor D .

From (5) is simple to see that as temperature vanishes ($D \rightarrow 0$) the unitary evolution is recovered. On the contrary, the case $\Omega \rightarrow 0$ (or $D \rightarrow \infty$) would correspond to *two* classical random walks. We note, however, that for the present two-body *quantum* problem, when $D/\hbar\Omega \gg 1$, the classical profile cannot be recovered because correlations between particles are induced from thermal bath \mathcal{B} . In addition, here we note that the initial condition of particles would be relevant for the calculation of the time-dependent bath-induced decoherence.

2.1 Solution for two QDW

We will solve this QME (5) with a localized initial condition in the Wannier lattice, i.e.,

$$\rho(0) = |s_1, s_2\rangle\langle s_1, s_2| = |\vec{0}\rangle\langle\vec{0}|. \quad (7)$$

The operational calculus in the QME will be done using Wannier vector states to evaluate elements of the density matrix $\rho(t)$.

To solve equation (5) we apply $|s_1, s_2\rangle$ from the right and $\langle s_1, s_2|$ from the left, then using equations (2) and (3) the evolution equation can be written in terms of the usual Wannier “*brac-ket*”. Therefore, we can introduce the discrete Fourier transform noting that a Fourier “*brac-ket*” is defined in terms of a Wannier basis for *two particles* in the form:

$$|k_1, k_2\rangle = \frac{1}{2\pi} \sum_{s_1, s_2 \in \mathcal{Z}} e^{ik_1 s_1} e^{ik_2 s_2} |s_1, s_2\rangle,$$

with $k_j \in (-\pi, \pi)$ and $s_1, s_2 \in$ integers. Thus finally the QME (5) can be written as:

$$\left\langle k_1, k_2 \left| \frac{d\rho}{dt} \right| k'_1, k'_2 \right\rangle = \mathcal{F}(k_1, k'_1, k_2, k'_2) \langle k_1, k_2 | \rho | k'_1, k'_2 \rangle,$$

here

$$\mathcal{F}(k_1, k'_1, k_2, k'_2) \equiv \{ \mathcal{F}^{(1)}(k_1, k'_1) + \mathcal{F}^{(1)}(k_2, k'_2) + 2D [\mathbf{C}(k_1, k'_2) + \mathbf{C}(k_2, k'_1) - \mathbf{C}(k_1, k_2) - \mathbf{C}(k'_1, k'_2)] \},$$

where

$$\mathcal{F}^{(1)}(k_2, k'_2) \equiv \left[\frac{-i}{\hbar} (\mathcal{E}_{k_2} - \mathcal{E}_{k'_2}) + 2D(\mathbf{C}(k_2, k'_2) - 1) \right],$$

is the one-particle infinitesimal generator in the Fourier representation [29],

$$\mathbf{C}(k_1, k_2) \equiv \cos(k_1 - k_2) \text{ and } \mathcal{E}_{k_i} \equiv \Omega \{1 - \cos k_i\}.$$

Note that $\mathcal{F}(k_1, k_1, k_2, k_2) = 0$ leading to a momentum-like conservation law: $\langle k_1, k_2 | \frac{d\rho(t)}{dt} | k_1, k_2 \rangle = 0$.

Elements of $\rho(t)$ can be calculated in the Wannier basis

$$|s_1, s_2\rangle = \frac{1}{2\pi} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} dk_1 dk_2 e^{-ik_1 s_1} e^{-ik_2 s_2} |k_1, k_2\rangle.$$

After some algebra and using Bessel’s function properties we can write an analytical formula for $\rho(t)$ in Wannier representation $\langle s_1, s_2 | \rho(t) | s'_1, s'_2 \rangle$ (to simplify the notation we use $t_\Omega \equiv \frac{\Omega t}{\hbar}$, $t_D \equiv 2Dt$ whenever it is necessary)

$$\begin{aligned} \langle s_1, s_2 | \rho(t) | s'_1, s'_2 \rangle &= i^{(s_1 - s'_1 + s_2 - s'_2)} e^{-2t_D} \sum_{\{n_1, n_2, n_3, n_4, n_5, n_6\} \in \mathcal{Z}} (-1)^{n_4 + n_5} \\ &\times J_{s_1 + n_1 + n_2 + n_5}(t_\Omega) J_{s'_1 + n_1 + n_3 + n_4}(t_\Omega) \\ &\times J_{s_2 + n_3 - n_5 + n_6}(t_\Omega) J_{s'_2 + n_2 - n_4 + n_6}(t_\Omega) \\ &\times \prod_{n_i=1}^6 I_{n_i}(t_D), \{s_j, s'_j\} \in \mathcal{Z} \end{aligned} \quad (8)$$

where J_n and I_n are Bessel’s functions of integer order $n \in \mathcal{Z}$. These functions satisfy that

$$J_{-n}(t) = (-1)^n J_n(t), \quad J_n(-t) = (-1)^n J_n(t),$$

and

$$I_{-n}(t) = I_n(t), \quad I_n(-t) = (-1)^n I_n(t).$$

This solution is symmetric under the exchange of particles¹ (therefore preserving the symmetry of the initial condition), is Hermitian and fulfills normalization in the lattice $\text{Tr}[\rho(t)] = \sum_{\{s_1, s_2\} \in \mathcal{Z}} \langle s_1, s_2 | \rho(t) | s_1, s_2 \rangle = 1, \forall t$; positivity is assured because the infinitesimal generator fulfills the structural theorem [3]. The probability of finding one particle in site s_1 and another in s_2 is given by the probability profile: $P_{s_1, s_2}(t) \equiv \langle s_1, s_2 | \rho(t) | s_1, s_2 \rangle$ and shows the expected reflection symmetry in the plane: $s_1 - s_2 = 0$.

In the case $D = 0$, i.e., a quantum closed system without dissipation, we recover the solution for two quantum walk: $\langle s_1, s_2 | \rho(t) | s'_1, s'_2 \rangle_{D=0} = \prod_{j=1}^2 i^{(s_j - s'_j)} J_{s_j}(t_\Omega) J_{s'_j}(t_\Omega)$, this means that from an uncorrelated initial condition $\rho(0)$, the solution $\rho(t \geq 0)_{D=0}$

¹ To prove the invariance under the exchange of particles: $\{s_1 \leftrightarrow s_2, s'_1 \leftrightarrow s'_2\}$, note that in equation (8) n_j are mute variables therefore we can use the change of variables $n_1 \leftrightarrow n_6, n_2 \leftrightarrow n_3$, finally $n_4 \leftrightarrow -n_4, n_5 \leftrightarrow -n_5$ to check this symmetry.

is written as the direct product of two independent quantum particles.

As we mentioned before a *classical* random walk regime [1,31] cannot be recovered. For $D \gg \Omega/\hbar$ the two-body density matrix is $\rho(t) \neq \rho_1(t) \otimes \rho_2(t)$, showing a complex pattern structure in terms of convolutions of classical profiles. From equation (8) it can be proved that when $D \gg \Omega/\hbar$ we get

$$\lim_{D \gg \Omega/\hbar} P_{s_1, s_2}(t) \neq P_{s_1}(t) \times P_{s_2}(t) = e^{-2tD} I_{s_1}(t_D) I_{s_2}(t_D),$$

here P_{s_j} is the classical probability profile for each particle. So a classical regime [for $t \rightarrow \infty$] cannot be obtained. This means that the profile for two DQW will not be a Gaussian bell-shape in 2D. In addition, it is intriguing to note that from the QME there exist an important competition between building correlations vs inducing dissipative decoherence.

Note that the one-particle density matrix is recovered tracing-out the degrees of freedom of the second one, say $j = 2$:

$$\rho^{(1)}(t) \equiv \text{Tr}_2[\rho(t)],$$

then

$$\begin{aligned} \langle s_1 | \rho^{(1)}(t) | s'_1 \rangle &= i^{(s_1 - s'_1)} e^{-tD} \\ &\times \sum_{n \in \mathcal{Z}} J_{s_1+n}(t\Omega) J_{s'_1+n}(t\Omega) I_n(tD), \end{aligned}$$

solution that indeed shows, for $D \gg \Omega/\hbar$, a random walk behavior for one particle [29]. In addition we note that in the lattice the classical random walk solution is $P_t(s) = e^{-2Dt} I_s(2Dt)$, and from this expression it is simple to get the Gaussian profile in the continuous limit [31].

3 Correlations and coherence in the infinite dimension Hilbert space

3.1 Purity

To measure the influence from \mathcal{B} into \mathcal{S} we study the Purity $\mathcal{P}_Q^{(2)}(t) \equiv \text{Tr}[\rho(t)^2]$ [4].

$$\begin{aligned} \mathcal{P}_Q^{(2)}(t) &= \text{Tr}[\rho(t)^2] = \sum_{s_1, s_2 = -\infty}^{\infty} \\ &\times \sum_{s'_1, s'_2 = -\infty}^{\infty} \langle s_1, s_2 | \rho(t) | s'_1, s'_2 \rangle \langle s'_1, s'_2 | \rho(t) | s_1, s_2 \rangle \\ &= e^{-8Dt} \sum_{m = -\infty}^{\infty} I_m(4Dt) \\ &\times \sum_{\alpha, \beta = -\infty}^{\infty} (-1)^{\alpha+\beta} I_\alpha(4Dt) I_\beta(4Dt) I_{\alpha+m}(4Dt) \\ &\times I_{\beta+m}(4Dt) I_{\alpha+\beta+m}(4Dt). \end{aligned} \quad (9)$$

We can prove that $\mathcal{P}_Q^{(2)}(t \geq 0) = 1$ for $D = 0$, and for $D \neq 0$ we get $\mathcal{P}_Q^{(2)}(t) \leq 1$ decreasing in the course of

time. Interestingly, for $D \neq 0$, $\mathcal{P}_Q^{(2)}(t)$ is different from the Purity for *two particles* with independent quantum baths, i.e., $\mathcal{P}_Q^{(2)}(t) \neq \mathcal{P}_Q^{(1)}(t) \mathcal{P}_Q^{(1)}(t)$, where

$$\mathcal{P}_Q^{(1)}(t) = e^{-4Dt} I_0(4Dt),$$

is the one-particle Purity (with independent bath [29]). Thus a common bath produces a difference in the total purity

$$\Delta \mathcal{P}_Q \equiv \mathcal{P}_Q^{(2)}(t) - \mathcal{P}_Q^{(1)}(t) \mathcal{P}_Q^{(1)}(t) \geq 0,$$

which shows the occurrence of bath-induced correlations.

An outstanding conclusion can be observed by introducing a *change of basis* in the representation of the two-particle density matrix $\rho(t) \equiv \rho(\Omega, D, t)$. Using the time-dependent unitary transformation:

$$\langle s_1, s_2 | U_1 | s'_1, s'_2 \rangle = i^{(s_1 + s_2 + s'_1 + s'_2)} J_{s_1 - s'_1} \left(\frac{\Omega t}{\hbar} \right) J_{s_2 - s'_2} \left(\frac{\Omega t}{\hbar} \right)$$

in equation (8) it is possible to prove that

$$U_1 \rho(\Omega, D, t) U_1^\dagger = \rho(\Omega = 0, D, t).$$

Thus, properties as Purity $\mathcal{P}_Q^{(2)}(t)$, Information Entropy $S(t) = -\text{Tr}[\rho \ln \rho]$ (von Neumann's entropy) can straightforwardly be shown in this new representation, see Figures 1a and 1b with and without a common bath. As $\rho_{\mathcal{S}+\mathcal{B}}(0)$ is a pure state, $S(t)$ is a good measure for the entanglement between the two particles with \mathcal{B} . We noted that even when the Purity is related to the Information Entropy, $\mathcal{P}_Q^{(2)}$ gives much insights: we see that $\rho(t)$ for two DQW's with a *common* bath the system has more Purity than the case of two DQW's with *independent* baths. The inset Figure 1b shows the difference $\Delta \mathcal{P}_Q$ from the mentioned cases showing a maximum of correlation for $t_D^{\text{max}} \approx 1.2$ before the dissipation wipes out the bath-induced coherence.

3.2 Quantum mirror correlations

Another measure to quantify the correlations *build up* between the particles, can be evaluated calculating correlation events for two particles. We define the total-mirror correlation $\mathcal{T}_{(1,2)}$, $\forall \{\Omega, D\}$, as:

$$\mathcal{T}_{(1,2)} = \sum_{s_1, s_2} \langle s_1, s_2 | \rho(t) | -s_1, -s_2 \rangle - \left(\mathcal{T}^{(1)} \right)^2,$$

where

$$\mathcal{T}^{(1)} = \sum_{s_1, s_2, s'_2} \langle s_1, s_2 | \rho(t) | -s_1, s'_2 \rangle = e^{-2Dt} I_0(2Dt).$$

The quantity $\mathcal{T}^{(1)}$ can be interpreted as the *one-particle* classical random walk return to the origin [31], to see this note that

$$\rho^{(1)}(t) = \text{Tr}_2[\rho(t)],$$

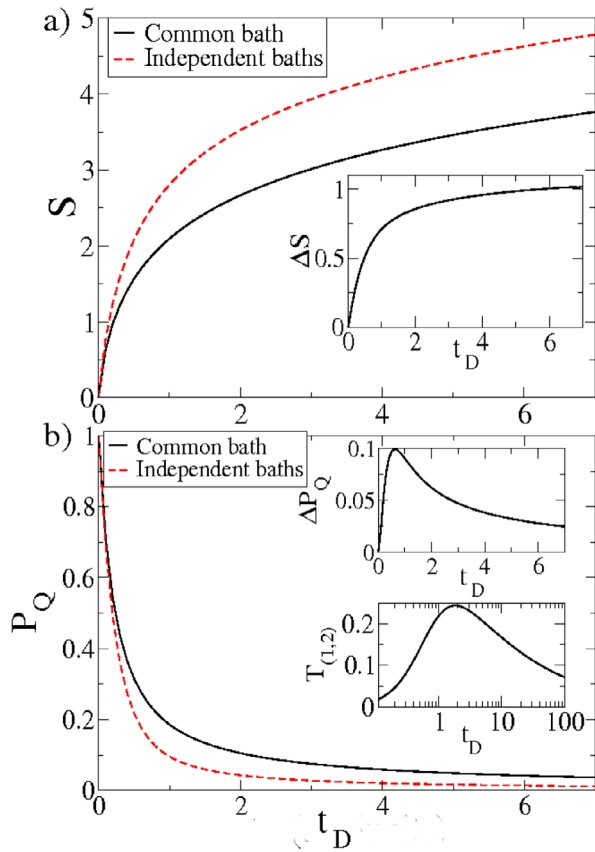


Fig. 1. (a) Information Entropy and (b) Purity for two different cases (using an initial condition as in Eq. (7)): two DQW's with a common \mathcal{B} and two DQW's with independent baths. Insets show the corresponding differences, and $\mathcal{T}_{(1,2)}$; all as a function of $t_D = 2Dt$.

and so

$$\sum_{s_1} \langle s_1 | \rho^{(1)}(t) | -s_1 \rangle = e^{-2Dt} I_0(2Dt).$$

In the inset of Figure 1b we plot the correlation $\mathcal{T}_{(1,2)}(t)$ showing that there is a time-scale when this quantum correlation reaches a maximum $t_D^{\max} \equiv 2Dt^{\max} \simeq 1.9 \dots$ before the long-time asymptotic regime $\sim 1/t$, characterizing the decoherence in the two-particles system.

3.3 Relative entropy of coherence

In this section, we will quantify the quantum coherence in our system. For such purpose we use an entropic measure of the quantum coherence called the Relative Entropy of Coherence [34,35].

For any quantum state $\rho = \rho(t)$ on the Hilbert space \mathcal{H} , the Relative Entropy of Coherence is defined as

$$C_{RE} = S(\rho_{diagonal}) - S(\rho),$$

where $S(\rho) = -\text{Tr}[\rho \ln \rho]$ is the von Neumann entropy. In [34], Baumgratz et al. shown that the Relative Entropy

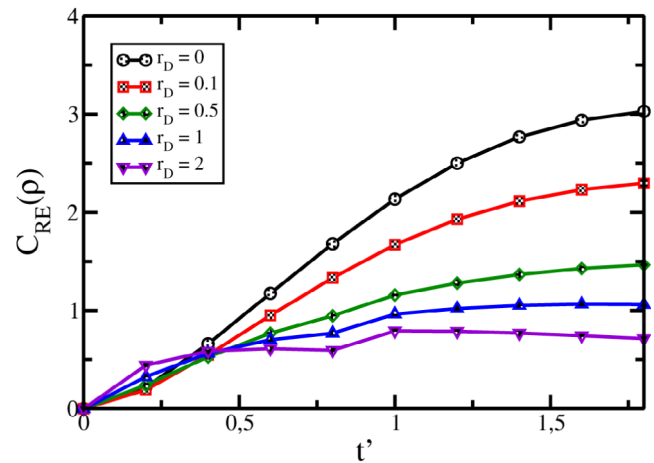


Fig. 2. Relative entropy of coherence for two particles with localized initial condition (see Eq. (7)) as function of $t' = t_\Omega \equiv \Omega t/\hbar$. This function shows a crossover at $t' \simeq 0.4$ as a function of time t' . The C_{RE} is calculated for different values of the dissipation parameter $r_D = \frac{2D}{\Omega/\hbar}$.

of Coherence is a good measure of the quantum coherence. In what follows we will use Wannier's basis to calculate C_{RE} . The results of this measure is shown in Figure 2. We have studied the C_{RE} as a function of $t' = t_\Omega = \frac{\Omega t}{\hbar}$ and we use several values of rescaled dissipation parameter $r_D \equiv \frac{2D}{\Omega/\hbar} = 0, 0.1, 0.5, 1, 2$. These results can also be used as an indicator that bath has created correlations between particles for $t' < \tau_c \approx 0.4$. For long times $t' > \tau_c$ the function C_{RE} decreases with increasing r_D ; this means that there is a strong competition between the bath-induced coherence and the inherent decoherence due to dissipation. Long-time values of C_{RE} are not plotted due to numerical computer limitations.

3.4 Quantum profile coherence

As before, let us use r_D the rate of energy scales $r_D \equiv \frac{2D}{\Omega/\hbar}$ and t' a dimensionless time (depending on the plotting we used t_Ω or t_D). In Figures 3b–3d we show the probability profile for having particles at the site s_1 and s_2 , i.e., $P_{s_1, s_2}(t' = t_\Omega)$ for different values of r_D (see Eq. (8)). Here, Figure 3b corresponds to the case when the two particles do not interact with the bath ($D = 0$), the inset shown the one-axis projection of one tight-binding quantum walk [29]. In Figure 3d $P_{s_1, s_2}(t' = t_D)$ corresponds to the high dissipative regime.

When $D > 0$ the probability profile is modified appearing interference patterns along of line $s_1 = s_2$, raising the value of the probability in the direction $s_1 = -s_2$ (conservation of total momentum), see Figure 3c. In the case $\Omega \rightarrow 0$ (or $r_D \gg 1$), the $P_{s_1, s_2}(t' = t_D)$ shows a different pattern signing the quantum nature in its profile, see Figure 3d. This is in contrast to the case of two particles with independent baths \mathcal{B}_1 and \mathcal{B}_2 in this case the probability profile is a Gaussian bell-shape as is shown in the inset. We remark that for two DQW

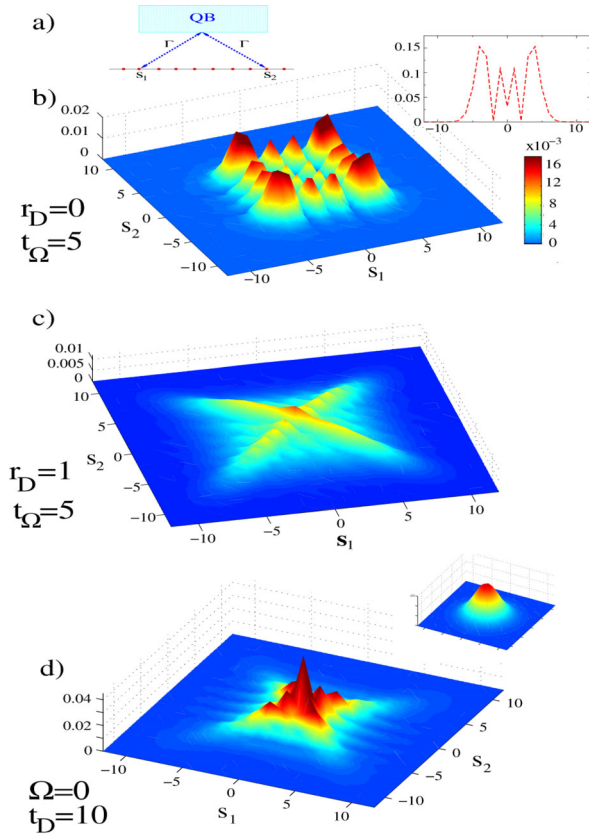


Fig. 3. (a) Representation of two DQW's interacting with \mathcal{B} . (b) Profile as a function of s_1 and s_2 . The inset shows the profile tracing out the second particle. (c) Here the pattern can be seen even when $D \neq 0$. (d) Profile for $r_D \gg 1$ (or $\Omega \rightarrow 0$). The inset shows the Gaussian bell-shape for two particles with independent baths. Blue indicates, roughly, the value zero while red a high value of probability.

with a common bath the probability profile can never be represented as a Gaussian distribution due to the bath-induced correlations.

3.5 Geometric quantum discord

To characterize the quantum correlations in the system we use the geometric quantum discord measure [36–39], which is easier to obtain instead of original quantum discord measure (which involves an optimization procedure [40,41]), and it has been proved to be a necessary and sufficient condition for non-zero quantum discord [36].

The geometric quantum discord (GQD) is defined as

$$D_G(\rho) = \min_{\chi \in \Omega_0} \|\rho - \chi\|^2, \quad (10)$$

where Ω_0 denotes the set of zero-discord states and $\|X - Y\|^2 = \text{Tr}(X - Y)^2$ is the square norm in the Hilbert-Schmidt space. Additionally, the lower bound of the GQD is calculated using the density operator, which is defined on a bipartite system (belonging to $H^a \otimes H^b$,

with $\dim H^a = m$ and $\dim H^b = n$) [36–39] as:

$$\rho = \frac{1}{mn} \left(\mathbf{I}_m \otimes \mathbf{I}_n + \sum_i x_i \tilde{\lambda}_i \otimes \mathbf{I}_n + \sum_j y_j \mathbf{I}_m \otimes \tilde{\lambda}_j + \sum_j t_{ij} \tilde{\lambda}_i \otimes \tilde{\lambda}_j \right),$$

here $\tilde{\lambda}_i, i = 1, \dots, m^2 - 1$ and $\tilde{\lambda}_j, j = 1, \dots, n^2 - 1$ are the generators of $SU(m)$ and $SU(n)$ respectively, satisfying $\text{Tr}(\tilde{\lambda}_i \tilde{\lambda}_j) = 2\delta_{ij}$, and \mathbf{I}_m is the identity operator in m -dimension. In this expression the vectors $\vec{x} \in R^{m^2-1}$ and $\vec{y} \in R^{n^2-1}$ of the subsystems A and B are given by:

$$x_i = \frac{m}{2} \text{Tr}(\rho \tilde{\lambda}_i \otimes \mathbf{I}_n) = \frac{m}{2} \text{Tr}(\rho_A \tilde{\lambda}_i)$$

$$y_j = \frac{m}{2} \text{Tr}(\rho \mathbf{I}_m \otimes \tilde{\lambda}_j) = \frac{n}{2} \text{Tr}(\rho_B \tilde{\lambda}_j),$$

and the correlation matrix $T \equiv [t_{ij}]$ is given by

$$T \equiv [t_{ij}] = \frac{mn}{4} \text{Tr}(\rho \tilde{\lambda}_i \otimes \tilde{\lambda}_j).$$

The lower bound of the GQD is calculated in the following form:

$$D_G(\rho) \geq \frac{2}{m^2 n} \left(\|\vec{x}\|^2 + \frac{2}{n} \|T\|^2 - \sum_{i=1}^{m-1} \eta_i \right), \quad (11)$$

where $\eta_i, i = 1, 2, \dots, m^2 - 1$ are eigenvectors of the matrix $(\vec{x}\vec{x}^t + \frac{2}{n} TT^t)$ arranged in non-increasing order [37].

3.5.1 Lattice bipartition, the qubit-qubit set

We need to define a procedure on the lattice in order to study the GQD (a similar approach has been done in [22]), in this context introducing a bipartition we will end with a *qutrit-qutrit system*.

In Figure 4a we show the mirror bipartition used in this work (a similar bipartition has been used for a spin system under the $SU(2)$ projection [42]). In the present case, tracing out (in the lattice) sites different from $\pm s$ it is possible to define a three-level system. Thus, in order to trace over all non-mirror sites ($\neq \pm s$) we defined the kets

$$|A\rangle \leftrightarrow |s\rangle$$

$$|B\rangle \leftrightarrow |-s\rangle$$

$$|\phi\rangle \leftrightarrow |s'\rangle, \quad s' \neq \pm s.$$

Then, the ket $|s_1, s_2\rangle$, representing a state of two particles, can be written in the form

$$|s_1, s_2\rangle = |\alpha\beta\rangle \otimes |R\rangle, \quad (12)$$

where $\{\alpha, \beta\} \in \{A, B, \phi\}$, and R is the complement, i.e., the set of all non-mirror sites.

Replacing (12) in (8) and tracing over $|\phi\rangle$ we obtain the density matrix ρ_{AB} . Thus ρ_{AB} turns to be a reduced (9×9) matrix, where the new ordered basis can be written as:

$$\{|AA\rangle, |AB\rangle, |A\phi\rangle, |BA\rangle, |BB\rangle, |B\phi\rangle, |\phi A\rangle, |\phi B\rangle, |\phi\phi\rangle\}.$$

In order to simplify this analysis we now reduce the representation to a *qubit-qubit* set, then we do not consider elements of the density matrix ρ_{AB} with vectors contribution:

$$\{|A\phi\rangle, |B\phi\rangle, |\phi A\rangle, |\phi B\rangle, |\phi\phi\rangle\},$$

i.e., representing the basis for the one-particle state and the empty state.

Therefore final density matrix reduces to a (4×4) matrix, within this approach we obtain the representation of a qubit-qubit system. Then, the lower bound of the GQD from equation (11) is reduced to:

$$D_G(\rho) \geq \frac{1}{4} \left(\|\vec{x}\|^2 + \|T\|^2 - k_{max} \right), \quad (13)$$

where k_{max} is the largest eigenvalue of $K = \|\vec{x}\|^2 + \|T\|^2$ [36]. Now, we calculate the total mirror contribution for the GQD defined as

$$D_G^T(\rho_{AB}) = \sum_{s=1}^{\infty} D_G^{(s)}(\rho_{AB}), \quad (14)$$

where $D_G^{(s)}(\rho_{AB})$ corresponds to equation (13) for a fixed value of s ($D_G^{(s)}(\rho_{AB})$ measures the quantum correlation between particles 1 and 2 to be confined at sites $\pm s$). We have plotted $D_G^T(\rho_{AB})$ as a function of time $t' = t\Omega$, for different values of $r_D \equiv \frac{2D}{\Omega/\hbar}$. In Figure 4b the GQD (lower bound given by Eq. (13)) is shown for different values of $r_D = 0.1, 0.5, 1, 2$.

One important conclusion from this result is that bath-induced correlations (between the particles) are in fact of quantum nature because $D_G^T(\rho_{AB}) > 0$ for almost all $t > 0$ and $r_D > 0$. Note that only if $r_D = 0$ the GQD vanishes at all times. From Figure 4b, we can see that the GQD shows a non-monotonic behavior as function of r_D then a characteristic time-scale τ_M can be defined signing its maximum value; note that as r_D decreases τ_M is delayed. In this figure we have not plotted the long-time behavior of GQD because we have numerical computed limitations.

4 Phase-space (lattice) representation

A important point of view is achieved if we introduce a quasi probability distribution function (pdf) for the infinite dimensional *discrete* Hilbert space associated to *two* DQW's. The crucial point in defining a Wigner function is to assure the completeness of the phase-space representation [43,44]. Then for this purpose we consider the *enlarged lattice* of integers (\mathcal{Z}) and semi-integers (\mathcal{Z}_2). Denoting

$$\vec{k} = (k_1, k_2), \quad \vec{x} = (x_1, x_2), \quad x_j \in (\mathcal{Z} \oplus \mathcal{Z}_2)$$

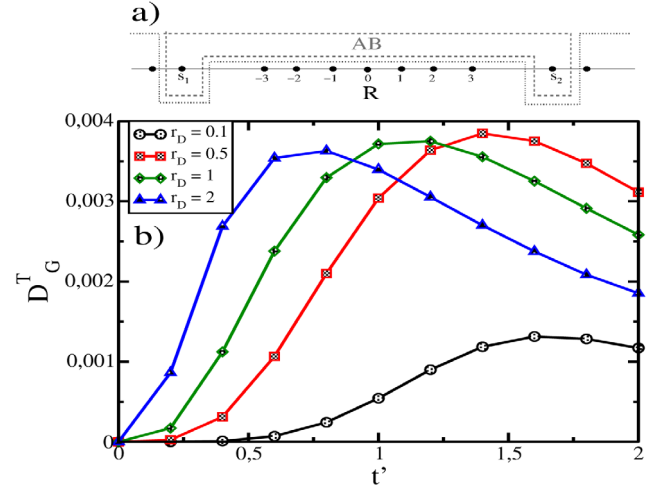


Fig. 4. (a) The bipartition to calculated the GQD. (b) The function $D_G^T(\rho_{AB})$ takes into account all the mirror contributions (qubit-qubit set) as defined in (14). A characteristic time τ_M can be defined when these correlations are maxima.

we define

$$W_t(\vec{k}, \vec{x}) = \sum_{x'_1, x'_2 \in (\mathcal{Z} \oplus \mathcal{Z}_2)} \langle x_1 + x'_1, x_2 + x'_2 | \rho_t | x_1 - x'_1, x_2 - x'_2 \rangle \frac{e^{-i2\vec{k} \cdot \vec{x}'}}{(2\pi)^2}, \quad (15)$$

which indeed fulfills

$$\sum_{\vec{x} \in (\mathcal{Z} \oplus \mathcal{Z}_2)} \int_{-\pi}^{\pi} d\vec{k} W_t(\vec{k}, \vec{x}) = 1$$

where $\rho_t \equiv \rho(t)$ is the two-body density matrix. Note that when $\rho(t)$ satisfies the exchange of particles symmetry (due to the particular initial condition we have used) our definition of the Wigner function fulfills also the invariance under exchange of particles but in the phase-space; i.e., under the exchange $x_1 \leftrightarrow x_2$ and $k_1 \leftrightarrow k_2$ (indicating that $W_t(\vec{k}, \vec{x})$ has a reflection symmetry in the planes: $x_1 - x_2 = 0$ and $k_1 - k_2 = 0$).

The present definition of $W_t(\vec{k}, \vec{x})$ can be proved to be equivalent to the definition using *phase-point operators* in finite systems [44–46]. We *remark* the prescription that

$$\langle \vec{x} | \rho_t | \vec{x}' \rangle = 0,$$

if some index $x_j \in \mathcal{Z}_2$ (this is so because Wannier's index are on \mathcal{Z}). Thus, our $W_t(\vec{k}, \vec{x})$ fulfills the fundamental conditions pointed out by Wigner et al. [43]: $\int \int d\vec{k} W_t(\vec{k}, \vec{x}) = \langle \vec{x} | \rho_t | \vec{x} \rangle \geq 0$ and $\sum_{\vec{x} \in (\mathcal{Z} \oplus \mathcal{Z}_2)} W_t(\vec{k}, \vec{x}) = \langle \vec{k} | \rho_t | \vec{k} \rangle \geq 0$. In addition, we noted that the *enlarged lattice* ($\mathcal{Z} \oplus \mathcal{Z}_2$) is the crucial key for a correct definition of a Wigner function. From the discrete Fourier transform we can obtain the *inverse* relation

on the Wannier lattice ($s_j \in \mathcal{Z}, \forall j = 1, 2$) as:

$$\langle s_1, s_2 | \rho_t | s'_1, s'_2 \rangle = \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} d\vec{k} W_t \times \left(k_1, k_2, \frac{s_1 + s'_1}{2}, \frac{s_2 + s'_2}{2} \right) e^{i\vec{k} \cdot (\vec{s} - \vec{s}')}.$$

Note that the inverse relation demands the necessity of a Wigner function defined on the *enlarged lattice*. After some algebra using solution (8) in definition (15) we get

$$W_t(\vec{k}, \vec{x}) = \frac{e^{-2tD}}{4\pi^2} (-1)^{2x_1+2x_2} \sum_{\{\alpha, \beta, q, n_2, n_3, n_5\} \in \mathcal{Z}} (-1)^{n_2+n_3+q} \times J_{2x_1+2\alpha-q}(-2t\Omega \sin k_1) J_{2x_2+2\beta+q}(-2t\Omega \sin k_2) \times I_{n_2}(tD) I_{n_3}(tD) I_{n_5}(tD) I_{n_2+n_5-\alpha}(tD) \times I_{n_3+n_5+\beta}(tD) I_{n_2+n_3+n_5-q}(tD) e^{iq(k_1-k_2)}. \quad (16)$$

As we commented before this solution is symmetric under exchange of particles because we have used a localized initial condition. In the case $D = 0$ we recover the non-dissipative description

$$W_t(\vec{k}, \vec{x})_{D=0} = \frac{(-1)^{2x_1+2x_2}}{4\pi^2} J_{2x_1} \times (-2t\Omega \sin k_1) J_{2x_2}(-2t\Omega \sin k_2)$$

representing two-independent quantum walks, and showing the possibility to be negative depending on the argument of the Bessel's functions and sites on the enlarged lattice. Thus, our Wigner function $W_t(\vec{k}, \vec{x})$ can be used to detect whether a point in phase-space has a pure quantum mechanics character or not. In Figure 5 we show several portraits, in particular it is clear to identify regions where $W_t(\vec{k}, \vec{x}) < 0$. Therefore we propose to use $W_t(\vec{k}, \vec{x})$ to measure the quantum to classical transition. In Figure 5 we show patterns for several values of $\Delta k \equiv k_1 - k_2$ and $t_D = 5$ on the *enlarged lattice* $\mathcal{Z} \oplus \mathcal{Z}_2$. On the other hand, putting $\Omega = 0$ in $W_t(\vec{k}, \vec{x})$ simplifies its analytical expression and shows also that there are domains where it is negative. This proves the quantum mechanics character of the bath-induced correlations between the two DQW, even in the large dissipative regime $\frac{2D}{\Omega/\hbar} \gg 1$. Note that the behavior of the *Negative Volume* of Wigner's function in phase-space can enlighten the understanding of the quantum character of the system behavior, as well as supporting the characterization of the typical *time-scale* for the coherence between particles, work along this line is in progress.

5 Discussions

We have analyzed two *free* spinless initially uncorrelated particles (in the lattice) in interaction with a common boson thermal bath \mathcal{B} . Even when the QME is a second

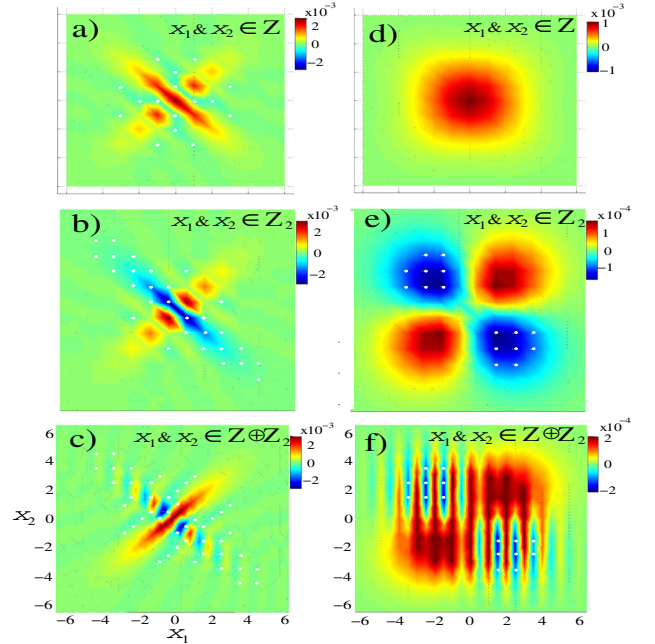


Fig. 5. Wigner function on the enlarged lattice for two DQW's as a function of $\{x_1, x_2\} \in (\mathcal{Z} \oplus \mathcal{Z}_2)$ for $t_D \equiv 2Dt = 5$ and two values of Δk . Due to the conservation of the pseudo-momentum Wigner's function does only depends on Δk . Domains where W_t is negative are shown in dark blue (white points are put to lighten when starts to be $W_t < 0$). In (a), (b), (c) $\Delta k = 0$, and (d), (e), (f) $\Delta k = \pi/3$.

order approach, the Markov approximation is enough to show bath-induced correlation among free particles. We have solved analytically the QME showing that if $D \neq 0$, we get $\rho(t) \neq \rho_1(t) \otimes \rho_2(t), \forall t > 0$, i.e., the time evolution is not a direct product of two independent particles if the temperature of the bath is non null. For $D = 0$ the probability profile $P_{s_1, s_2}(t) \equiv \langle s_1, s_2 | \rho(t) | s_1, s_2 \rangle$ is ballistic and starts to be modified by the presence of dissipation $D > 0$, showing a *X-form* pattern. In the case of large dissipation, $r_D \equiv \frac{2D}{\Omega/\hbar} \gg 1$, this structure is accentuated and additional interferences are observed. Several correlations measures: $\mathcal{T}_{(1,2)}$, Purity and Relative Entropy of Coherence C_{RE} have been analyzed showing a degree of coherence between particles, these correlations are induced by the common bath \mathcal{B} despite the presence of dissipation for temperature $T \neq 0$. \mathcal{P}_Q , Mirror Correlation $\mathcal{T}_{(1,2)}$ and GQD have been used to show the existence of a *time-scale* when the quantum correlations reach a maximum. All these measured of correlations have also been indirectly supported by an independent analysis using a Wigner function defined on the enlarged lattice of integers and semi-integers ($\mathcal{Z} \oplus \mathcal{Z}_2$); showing that this function is negative in some domains of phase-space. Thus we propose to use the total *negative volume* of the Wigner function in phase-space to characterize the quantum to classical transition in this type of many-body system, work along this line is in progress.

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Author contribution statement

Both authors contributed equally to this paper.

Appendix A: Semigroup for two distinguishable quantum random walk

Starting from the total Hamiltonian $H_{\mathcal{T}}$ and eliminating the bath variables (in the Markov approximation), the Kossakowski-Lindblad infinitesimal generator [3] can be written in the form

$$\mathcal{KL}[\bullet] = -\frac{i}{\hbar} [H_{eff}, \bullet] + F[\bullet] - \frac{1}{2} \{F^*[\mathbf{1}], \bullet\}_+, \quad (\text{A.1})$$

where H_{eff} is the effective Hamiltonian, $\frac{1}{2}F^*[\mathbf{1}]$ can be regarded as a dissipative operator, and $F^*[\bullet]$ the fluctuating superoperator ($F^*[\bullet]$ is the dual operator of $F[\bullet]$, and $\{\bullet, \bullet\}_+$ the anticommutator). Using a separable initial condition for the total density matrix $\rho_{\mathcal{T}}(0) = \rho(0) \otimes \rho_B^e$, and working in a second order approximation we can write (ρ_B^e is the thermal density matrix of the bath at temperature T)

$$\begin{aligned} H_{eff} &= H_S - i\frac{1}{2\hbar} \int_0^\infty d\tau \text{Tr}_B ([H_{SB}, H_{SB}(-\tau)] \rho_B^e), \\ F[\rho(t)] &= \left(\frac{1}{\hbar}\right)^2 \int_0^\infty d\tau \text{Tr}_B [H_{SB}\rho(t) \otimes \rho_B^e H_{SB}(-\tau) \\ &\quad + H_{SB}(-\tau)\rho(t) \otimes \rho_B^e H_{SB}], \end{aligned}$$

where $H_{SB}(-\tau) = e^{-i\tau(H_S+H_B)/\hbar} H_{SB} e^{i\tau(H_S+H_B)/\hbar}$ [3,20]. Noting that a_{12} and a_{12}^\dagger are constant in time, $[a_{12}, a_{12}^\dagger] = 0$ and using the full expressions of H_S, H_B and H_{SB} , after some algebra we can write

$$F[\bullet] = \frac{\pi 4\Gamma^2}{2\hbar/k_B T} [a_{12} \bullet a_{12}^\dagger + a_{12}^\dagger \bullet a_{12}], \quad (\text{A.2})$$

where $\pi\Gamma^2 k_B T/\hbar$ is a dissipative constant (here we have used the Ohmic approximation for the *strength function* $g(\omega)$ of the bath, i.e., $g(\omega) = \sum_k |v_k|^2 \delta(\omega - \omega_k) \propto \omega$, if $0 < \omega < \tilde{\omega}_c$). In a similar way the effective Hamiltonian can be calculated given

$$H_{eff} = H_S - \omega_c \hbar a_{12} a_{12}^\dagger,$$

here $\omega_c \equiv 2\tilde{\omega}_c \Gamma^2$ is an upper bound frequency.

Using these expressions we can write down the QME (5) in the form

$$\dot{\rho} = L[\rho], \quad L[\bullet] \equiv -\frac{i}{\hbar} [H_{eff}, \bullet] + F[\bullet] - \frac{1}{2} \{F[\mathbf{1}], \bullet\}_+,$$

then the solution can be written in the formal form:

$$\rho(t) = \sum_{m=0}^{\infty} \int_0^t dt_m \int_0^{t_m} dt_{m-1} \cdots \int_0^{t_2} dt_1 \{ \mathcal{L}_0(t-t_m) F[\bullet] \mathcal{L}_0(t_m-t_{m-1}) \cdots F[\bullet] \mathcal{L}_0(t_1) \} \rho(0), \quad (\text{A.3})$$

where it is evidenced that the system is exposed to a succession of quantum jumps associated to the superoperator $F[\bullet]$, and intercalating a smooth evolution characterized by

$$\mathcal{L}_0(t)\rho = \exp \left\{ \left(-\frac{i}{\hbar} [H_{eff}, \bullet] - \frac{1}{2} \{F[\mathbf{1}], \bullet\}_+ \right) t \right\} \rho.$$

This picture allows to generalize the description of a QDW into a non-Markovian evolution using the CTRW approach [30,31]. See also a related contribution, in the present issue, for describing completely positive quantum maps in the context of the *Renewal theory* [32].

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