Non-equilibrium transition from dissipative quantum walk to classical random walk

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Abstract
We have investigated the time evolution of a free particle in interaction
with a phonon thermal bath, using the tight-binding approach. A dissipative
quantum walk can be defined and many important non-equilibrium decoherence
properties can be investigated analytically. The non-equilibrium statistics of
a pure initial state have been studied. Our theoretical results indicate that
the evolving wave-packet shows the suppression of Anderson's boundaries
(ballistic peaks) by the presence of dissipation. Many important relaxation
properties can be studied quantitatively, such as von Neumann's entropy and
quantum purity. In addition, we have studied Wigner's function. The time-
dependent behavior of the quantum entanglement between a free particle—in
the lattice—and the phonon bath has been characterized analytically. This result
strongly suggests the non-trivial time dependence of the off-diagonal elements
of the reduced density matrix of the system. We have established a connection
between the quantum decoherence and the dissipative parameter arising
from interaction with the phonon bath. The time-dependent behavior of
quantum correlations has also been pointed out, showing continuous transition
from quantum random walk to classical random walk, when dissipation
increases.

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(Some figures may appear in colour only in the online journal)

1. Introduction

The need to understand the evolution of a wave-packet (for instance, one particle in a one-
dimensional lattice) has been motivated by many problems in solid-state physics [1], quantum
information [2], quantum open systems [3–6] and quantum optics [5, 7], among others. In
solid-state physics, in particular, the spread of a wave-packet from a highly localized initial
state in the tight-binding lattice approximation [1, 8] has drawn the attention of many authors
[9, 10]. Interestingly, the concept of quantum walk (QW), borrowed from classical statistics

[11–14], has the same properties as a tight-binding free particle [14, 15]. Two kinds of QW are considered in the literature: discrete-time quantum-coined walk [7, 9, 11, 13, 16–23] and continuous-time QW [10, 14, 15, 24–27]. In the former (proposed by Aharonov *et al* [11]), a two-level state, the so-called coin, rules the unitary discrete-time evolution of a particle moving in a lattice. On the other hand, the evolution of the particle in the continuous-time QW is determined by a tight-binding-like Hamiltonian [15, 27]. It is not difficult to see, by simple comparison, that a mapping between the *tight-binding* Hamiltonian and the QW model can be established (see appendix A).

There are some important differences between a classical random walk (CRW) and a QW and these differences are well known in the literature [6, 9, 10, 28]. The most important of these differences is the fact that for a tight-binding free particle the deviation $\sigma(t)$ of the wave-packet becomes linear in time $\sigma(t) \sim t$ (QW), in contrast to the CRW result that becomes similar to $\sigma(t) \sim \sqrt{t}$. This issue can be resolved straightforwardly by analyzing, in the Heisenberg picture, the time evolution of the second moment of the position of the free particle [26]. QWs have been studied for possible applications in quantum information and quantum computation algorithms [2, 13]. Discrete-time evolution in random media has recently been used to study entanglement and quantum correlations in order to understand the role of noise and the mechanism of decoherence between the internal and spatial degrees of freedom in a QW [17].

The study of a QW subjected to different sources of decoherence is an active topic that has been considered by several authors, in particular, due to their interest in understanding laser cooling experiments [29], modeling blinking statistics [30] and carrying out quantum simulations [18]. Experimental study of quantum decoherence in discrete-time QW using single photons in the space was performed in [19]. These authors considered pure dephasing as a decoherence mechanism and they could explore the quantum to classical transition by means of tunable decoherence. In other theoretical studies [10, 16, 20–22], the authors analyzed discrete-time and continuous-time QW in a random environment, and they could also study the quantum–classical transition. In [31], the authors study QW with decoherence by analyzing a non-unitary evolution in QW. Experimental analysis of QW in a random environment led to the study of quantum optical devices [7, 9, 23–25]; interestingly, these experiments also show the non-classical behavior in dissipative QW (DQW).

In classical statistics and via the central limit theorem, the Gaussian distribution plays a fundamental role in all random walks with finite mean-square displacement per step [6, 28]. In quantum statistics, however, this analysis is much more complex because quantum thermal average must be taken using the reduced density matrix. On the other hand, in the Markov approximation, the time evolution for the reduced density matrix requires a much more complex infinitesimal generator, and in fact this generator has been studied extensively, for many years, and is nowadays called the Kossakoski–Lindblad generator [32, 33]. One of the most interesting facts that distinguishes quantum mechanics from classical mechanics is the coherent superposition of distinct physical states. Many of the non-intuitive aspects of the quantum theory of matter can be traced to the coherent superposition feature. Related to this issue, an interesting question arises: how does coherent superposition operate in the presence of dissipation? These subjects have been important issues of research since the pioneer works of Feynman and Vernon [34, 35] and Caldeira and Leggett [36], among others, see for example [5, 6, 37–39].

An important fact in modeling a realistic QW is the inclusion of the quantum thermal bath $\mathcal{B}$ from the very beginning in order to get a dissipative open system [4–6]. To emphasize this fact we call this continuous-time model a DQW, and this may be a mechanism of decoherence in a QW. Nevertheless, there are many other mechanism of decoherence, see

for example [31]. To our knowledge this pioneer problem was well posed in van Kampen's paper [12], but many other related approaches have also been presented in the literature [15, 40]. The propagation of photons in waveguide lattices has been studied in recent years [24, 25], and they are possible scenarios where our present results can be applied.

In this paper, we study an open system in the Markov approximation to continuous time [26, 41], i.e. a quantum mechanical particle that moves along a lattice by hopping while interacting with a thermal phonon bath $\mathcal{B}$. We have chosen an interaction Hamiltonian with the bath in such a way that this interaction produces the hopping in the tight-binding particle. Therefore, we highlight some of the issues of interpretation of the coherent superposition by tackling a soluble hopping model. The asymptotic long-time regime of the quantum probability, Wigner's function, quantum entropy, quantum purity, etc are characterized as a function of the dissipation. The long-time decoherent behavior is also explained in terms of the present dissipative hopping model. This model analytically reproduces the (non-equilibrium) continuous transition from DQW to CRW when the diffusion coefficient goes to infinity (i.e. when the temperature of the bath $T \to \infty$).

1.1. A tight-binding open model

We have considered a free-particle model (tight-binding approximation, for example see [8]) constrained to a one-dimensional regular and infinity lattice (in one band side) in interaction with a thermal bath of phonon $\mathcal{B}$. The total Hamiltonian for this problem can be written in the form [12]

$$H_{\mathcal{T}} = \left(E_0 \mathbf{1} - \Omega \frac{a + a^\dagger}{2} \right) + \sum_{\nu=1}^{2} V_\nu \otimes B_\nu + H_{\mathcal{B}}. \tag{1}$$

The first term corresponds to the *tight-binding* Hamiltonian H_S, where a and $a^\dagger$ are translational operators in the Wannier bases $|s\rangle$ (it is easy to write these operators in second quantization, for more details see appendix A) and $\mathbf{1}$ is the identity operator. The second term is the interaction Hamiltonian and corresponds to a linear coupling between phonon operators $B_1 = B_2^\dagger = \sum_k v_k \mathcal{B}_k$ and system operators $V_1 = V_2^\dagger = \hbar \Gamma a$, here $\Gamma > 0$ is the coupling parameter. The third term is the phonon Hamiltonian written in terms of boson operators $\sum_k \hbar \omega_k \mathcal{B}_k^\dagger \mathcal{B}_k$ [26, 41, 42]. Here E_0 is the *tight-binding* energy of site and Ω is the associated next-neighbor hopping energy.

The quantum master equation (QME) for our DQW model can be obtained by eliminating the variables of the quantum thermal bath and assuming for the initial condition of the total density matrix $\rho_T(0) = \rho(0) \otimes \rho_{\mathcal{B}}^{\text{eq}}$, where $\rho_{\mathcal{B}}^{\text{eq}}$ is the equilibrium density matrix of the quantum bath $\mathcal{B}$. Then, in the Markov approximation, using $[a, a^\dagger] = 0$ and $a^\dagger a = \mathbf{1}$, the evolution equation for the reduced density matrix is [26, 41]

$$\dot{\rho} \equiv \frac{d\rho}{dt} = \frac{-i}{\hbar} [H_{\text{eff}}, \rho] + D\left(a\rho a^\dagger + a^\dagger \rho a - 2\rho \right), \tag{2}$$

with a trivial effective Hamiltonian: $H_{\text{eff}} = H_S - \hbar \omega_c \mathbf{1}$. The diffusion constant is given in terms of the quantum thermal bath temperature and the coupling constant in the form

$$D \propto \Gamma^2 k_B T / \hbar,$$

the additive energy $\hbar \omega_c$ is related to the Caldeira and Legett frequency cut-off in the ohmic approximation [36]. For simplicity, we can add an additive constant to the *tight-binding* Hamiltonian $-E_0 + \omega_c \hbar + \Omega$. This assumption does not change the general results and finally we can write

$$H_{\text{eff}} = \Omega \left(\mathbf{1} - \frac{a + a^\dagger}{2} \right), \tag{3}$$

as was presented in [12, 26, 41]. It can be noted from equation (2) that as $D \to 0$ ($T \to 0$), the von Neumann equation is recovered (unitary evolution).

1.1.1. On the second moment of the DQW. From the QME equation (2), we can obtain the dynamics of any operator; in particular, here we are interested in the evolution of the dispersion of the position operator $\mathbf{q}$, which in the Wannier basis has the matrix elements (s is an eigenvalue of $\mathbf{q}$)

$$\langle s \,|\mathbf{q}|s' \rangle = s \, \delta_{s,s'}, \tag{4}$$

note that $\mathbf{q}$ is defined as a dimensionless position operator with lattice parameter $\epsilon = 1$. Then the quantum thermal time evolution of the first and second moments can be calculated straightforwardly. In the Heisenberg representation, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{q}(t) = \frac{-\mathrm{i}}{\hbar}\big[\mathbf{q}, H_{\mathrm{eff}}\big] \tag{5}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{q}^2(t) = \frac{-\mathrm{i}}{\hbar}\big[\mathbf{q}^2, H_{\mathrm{eff}}\big] + 2D\mathbf{1}, \tag{6}$$

where we have used that $[\mathbf{q}, H_{\mathrm{eff}}] = \frac{\Omega}{2}\left(a - a^\dagger\right)$ and that $a(t) = a(0)$, $a^\dagger(t) = a^\dagger(0)$, then we obtain for the time evolution of the position operator

$$\mathbf{q}(t) = \frac{-\mathrm{i}\Omega}{2\hbar}(a - a^\dagger)t + \mathbf{q}(0).$$

It is simple to realize, just from a physical point of view, why there is no dissipative term in the equation of motion for $\mathbf{q}(t)$. Taking the thermal average in equation (5) we obtain $\frac{\mathrm{d}}{\mathrm{d}t}\langle\mathbf{q}(t)\rangle = \frac{\Omega}{\hbar}\sum_{s=-\infty}^{s=\infty}\mathrm{Im}[\rho_{s,s-1}(t)]$, then introducing the explicit solution for the density matrix, equation (13), and using the properties of the Bessel function (with integer indices) $\sum_{s=-\infty}^{s=\infty} J_{s+n}(x)J_{s+m}(x) = \delta_{n,m}$. We obtain that $\frac{\mathrm{d}}{\mathrm{d}t}\langle\mathbf{q}(t)\rangle = 0$ indicating the conservation of reflection symmetry at the localized initial condition; otherwise, if $\frac{\mathrm{d}}{\mathrm{d}t}\langle\mathbf{q}(t)\rangle \neq 0$, this would destroy the reflection symmetry principle.

The quantum thermal statistical average—of any operator—in the Heisenberg picture can be written as $\langle\mathbf{A}(t)\rangle = \mathrm{Tr}\,[\mathbf{A}(t)\rho(0)]$. Then for the variance of the DQW we obtain

$$\sigma(t)^2 = \big\langle\mathbf{q}(t)^2\big\rangle - \big\langle\mathbf{q}(t)\big\rangle^2 = \frac{1}{2}\left(\frac{\Omega t}{\hbar}\right)^2 + 2Dt, \tag{7}$$

which is the expected dissipative result [6, 12, 26, 41]. From equations (5) and (6), it is possible to see that von Neumann's term gives a contribution of the form $\propto t^2$ for the time evolution of the second moment, this is a well-known quantum result. In fact for the null dissipation case, $D = 0$, we obtain that Anderson's boundaries (ballistic peak) movement is controlled by the linear law of the deviation of the wave-packet:

$$\sigma(t) = \sqrt{\big\langle\mathbf{q}(t)^2\big\rangle - \big\langle\mathbf{q}(t)\big\rangle^2} = \frac{1}{\sqrt{2}}\frac{\Omega t}{\hbar}, \text{ if } D = 0.$$

Therefore, we can associate the quantity $V_A = \frac{1}{\sqrt{2}}\frac{\Omega}{\hbar}$ with the velocity of Anderson's boundaries in a one-dimensional regular lattice.

In the appendix C, we have calculated the second moment of the position operator by using the characteristic function, which is useful for calculating all quantum thermal moments.

In the next section we will present, in detail, results concerning the probability profile of our quantum open model ($D \neq 0$), i.e. *a dissipative tight-binding free particle*. We will study the time evolution of the reduced density matrix [42, 43], characterize its decoherence, and solve, analytically, some correlation functions associated with the coherent superposition feature.

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2. Time evolution of the DQW

2.1. General properties

In order to consider the evolution of our free particle in interaction with the quantum thermal bath $\mathcal{B}$, we have to solve the QME, equation (2), for any time. This can be done in the Fourier representation. Let the Fourier '*bra-ket*' be defined in terms of the Wannier '*bra-ket*' in the form

$$|k\rangle = \frac{1}{\sqrt{2\pi}} \sum_{s=-\infty}^{\infty} e^{iks} |s\rangle,$$

$$\langle k| = \frac{1}{\sqrt{2\pi}} \sum_{s=-\infty}^{\infty} e^{-iks} \langle s|.$$

Then, the QME adopts an explicit form:

$$\langle k_1|\dot{\rho}|k_2\rangle = \left[\frac{-i}{\hbar}(\mathcal{E}_{k_1} - \mathcal{E}_{k_2}) + 2D(\cos(k_1 - k_2) - 1) \right] \langle k_1|\rho|k_2\rangle, \tag{8}$$

where $\mathcal{E}_k = \Omega \{1 - \cos k\}$. Note that the diagonal elements $\rho_{k,k}(t) \equiv \langle k|\rho(t)|k\rangle$ are constant in time, $\dot{\rho}_{k,k}(t) = 0$, for example, for a localized initial condition $\rho(0) = |s_0\rangle\langle s_0|$ (with $s_0 = 0$) we obtain

$$\rho_{k,k}(t) = \rho_{k,k}(0) = \frac{1}{2\pi}, \quad \forall t, \tag{9}$$

even so, we can define a pseudo-momentum operator $\mathbf{p} \equiv \frac{m}{i\hbar}[q, H_s]$, where m represents the mass of the free particle in the model. We can calculate any moment of the pseudo-momentum operator, $\langle \mathbf{p}^j \rangle = \text{Tr}[\mathbf{p}^j \rho(t)]$ for $j = 1, 2, \ldots$. For the case $j = 1$, we obtain $\langle \mathbf{p} \rangle = 0$ and for $j = 2$, we obtain $\langle \mathbf{p}^2 \rangle = \frac{1}{2}(\frac{\Omega}{\hbar})^2 m^2$. Then, we can define the quantum thermal second moment of the velocity $\mathbf{v}$ in the following way: $\langle \mathbf{v}^2 \rangle = \frac{1}{2}(\frac{\Omega}{\hbar})^2$ and so we re-obtain the velocity of Anderson's boundaries $V_A = \frac{1}{\sqrt{2}}\frac{\Omega}{\hbar}$ (see subsection on the second moment of the DQW).

To solve equation (8) we define the function:

$$\mathcal{F}(k_1, k_2) = i\frac{\Omega}{\hbar}(\cos(k_1) - \cos(k_2)) + 2D(\cos(k_1 - k_2) - 1), \tag{10}$$

the general solution of the QME can be written as

$$\langle k_1|\rho(t)|k_2\rangle = \rho(0)_{k_1 k_2} \exp(\mathcal{F}(k_1, k_2)t). \tag{11}$$

In order to study the suppression of Anderson's boundaries by the presence of dissipation, it is convenient to go back to the Wannier representation $(|s\rangle = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} dk\, e^{-iks} |k\rangle)$. Adopting equation (9), as initial condition for the density matrix, we obtain

$$\langle s_1|\rho(t)|s_2\rangle = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk_1 \int_{-\pi}^{\pi} dk_2\, e^{i(k_1 s_1 - k_2 s_2)} \langle k_1|\rho(t)|k_2\rangle$$

$$= \left(\frac{1}{2\pi}\right)^2 \int_{-\pi}^{\pi} dk_1 \int_{-\pi}^{\pi} dk_2\, e^{[i(k_1 - k_2)(s_1 - s_2)]} e^{\mathcal{F}(k_1, k_2)t}. \tag{12}$$

We can solve equation (12) analytically if we consider Bessel's function properties: $e^{iz\cos\theta} = \sum_{n=-\infty}^{\infty} i^n J_n(z) e^{in\theta}$; $e^{z\cos\theta} = \sum_{n=-\infty}^{\infty} I_n(z) e^{in\theta}$, where J_n and I_n are Bessel functions of integer order. Using the following relations $J_{-n}(x) = (-1)^n J_n(x)$, $J_n(-x) = (-1)^n J_n(x)$ and $I_{-n}(x) = I_n(x)$, $I_n(-x) = (-1)^n I_n(x)$, where n is an integer [44, 45], we have obtained an analytical expression for $\langle s_1|\rho(t)|s_2\rangle$ (for more details, see appendix B):

$$\langle s_1|\rho(t)|s_2\rangle = i^{(s_1 - s_2)} e^{-2Dt} \sum_{n=-\infty}^{\infty} J_{s_1+n}\left(\frac{\Omega t}{\hbar}\right) J_{s_2+n}\left(\frac{\Omega t}{\hbar}\right) I_n(2Dt). \tag{13}$$

Using $\sum_{n=-\infty}^{\infty} J_n^2(x) = 1$ and $\sum_{-\infty}^{\infty} I_n(x) = e^x$ [44], we can check that equation (13) fulfils the normalization condition $\text{Tr}[\rho(t)] = \sum_{s=-\infty}^{\infty} \langle s|\rho(t)|s\rangle = 1, \forall D$, and the probability of finding the particle in the site s in the lattice is

$$P_s(t) \equiv \langle s|\rho(t)|s\rangle = e^{-2Dt} \sum_{n=-\infty}^{\infty} \left[J_{s+n}\left(\frac{\Omega t}{\hbar}\right) \right]^2 I_n(2Dt), \ DQW. \qquad (14)$$

It is straightforward to note that equation (13) contains all the information concerning the transition from DQW to CRW. In fact, this transition is a genuine non-equilibrium one because any behavior characterizing the quantum to classical transition will be given in terms of the time evolution of the density matrix, which of course is not a Gibbsian density matrix [3–5].

If $D = 0$ (without dissipation, i.e. a closed system), we recover the QW and in this case the matrix elements $\langle s_1|\rho(t)|s_2\rangle$ reduce to the form (using $I_n(0) = \delta_{n,0}$, where n is an integer)

$$\langle s_1|\rho(t)|s_2\rangle_{D=0} = i^{(s_1-s_2)} J_{s_1}\left(\frac{\Omega t}{\hbar}\right) J_{s_2}\left(\frac{\Omega t}{\hbar}\right), \ QW. \qquad (15)$$

In the case $D \to \infty$, we can re-obtain exactly the classical probability [6, 28], where the off-diagonal elements of $\rho(t)$ in Wannier basis are equal to zero. Alternatively, consider the limits $\Omega \to 0$ and $\hbar \to 0$ in such a way that

$$\lim_{\Omega \to 0, \hbar \to 0} \frac{\Omega}{\hbar} \to 0,$$

then from equation (14) and using $J_{s+n}(0) = \delta_{s+n,0}$, where $s + n$ is an integer it follows (for any finite time t) that

$$\lim_{\Omega \to 0, \hbar \to 0} \langle s|\rho(t)|s\rangle \to e^{-2Dt} \sum_{n=-\infty}^{\infty} [\delta_{s,-n}]^2 I_n(2Dt) = e^{-2Dt} I_s(2Dt),$$

which is just the probability of the CRW, i.e.

$$P_s(t) = e^{-2Dt} I_s(2Dt), \ CRW. \qquad (16)$$

We note from equation (16), when $t \to \infty$ that we re-obtain the well-known Gaussian asymptotic scaling for the CRW probability $P_s(t \to \infty) \to \frac{t^{-1/2}}{\sqrt{4\pi D}}$ (we have used the asymptotic limit of $I_n(x) \approx \frac{e^x}{\sqrt{2\pi x}}$, for $x \to \infty$ [44]).

Here, we have considered it appropriate to define a new parameter such that $r_D = \frac{2D}{\Omega/\hbar}$ (rate of characteristic energy scales in the system) and $t' = \frac{\Omega}{\hbar} t$ a dimensionless time, in order to plot the analytical expression (14). In figure 1, we show the probability at the site s $P_s(t) = \langle s|\rho(t)|s\rangle$, for different values of the dissipative parameter r_D (see, equation (14)). Similar plots for the probability profile in the presence of dissipation have been analyzed by Esposito et al [15].

Note from figure 1 that for $D = 0$ ($r_D = 0$), the system is not interacting with the phonon bath; in this case, we get a closed system, and therefore the evolution of the wave-packet is not diffusive but is ballistic, equation (15). So for $t' = 31.8$ we observe two maximum peaks in $s_p \approx \pm 29$, which correspond to ballistic peaks (Anderson's boundaries), and far away from these peaks for $|s| > s_p$ the probability quickly goes to zero. In the case that $|s| < s_p$, we easily see oscillatory behavior because of the quantum behavior of the system. If the dissipative term is small $r_D \ll 1$ ($r_D = 0.05$) the oscillatory behavior starts to decrease and when the dissipation is of the order of the hopping energy ($r_D = 1$) or larger ($r_D = 5, 10$, see figure1), the dissipation dominates in the system and the quantum character vanishes. In this case, the wave-packet tends to a Gaussian form. This is the regimen for the CRW, equation (16).

In the remainder of the paper, we are going to study the probability profile of the DQW, the quantum purity, the Wigner function and von Newmann's entropy as a function of the
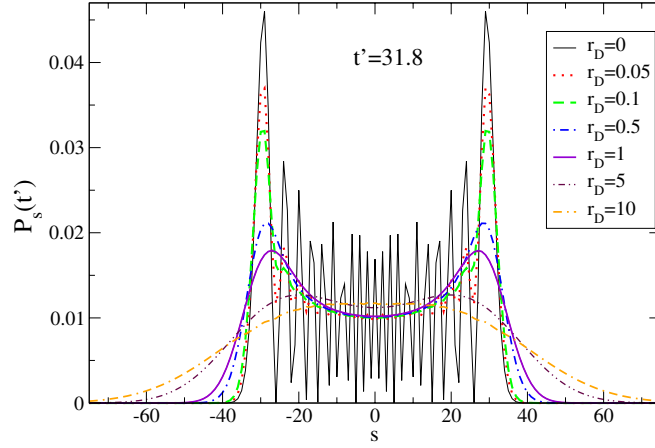
Figure 1. Probability $P_s(t')$ for an initial condition $\rho(0) = |s_0\rangle\langle s_0|$ (where $s_0 = 0$) as a function of position s, for $r_D = 0, 0.1, 0.5, 1, 5, 10$ and $t' = 31.8$, where we have defined the new variables $r_D = \frac{2D}{\Omega/\hbar}$ and $t' = \frac{\Omega}{\hbar}t$ (dimensionless time).

dissipative parameter r_D. In the Wigner section, we are also going to introduce a criterion to describe the quantum–classical transition (see inset of figure 5). In a future work, we will present analytical and numerical results such as the concurrence, negativity, etc as a function of r_D in order to study the decoherence and the entanglement in a bipartite system related to our DQW.

In figure 2, we show the same facts as in figure 1 (for some values of r_D) but in three dimensions (3D); i.e. we have included an extra axis for the time t' (this kind of graphic representation is usually called quantum carpet). We cut the axis of the probability for convenience (for example we do not show the probability for $t' = 0$, $P_s(0) = 1$). In this quantum carpet, we observe the transition from quantum regimen (figure 1 (a)) to classical regimen (figure 1 (d)). Oscillatory behavior for small values of D ($r_D \ll 1$) is observed, and the oscillations in the probability start to disappear when r_D is larger than one.

On the other hand, the quantum purity [2] ($\mathcal{P}_Q(t) \equiv \text{Tr}[\rho(t)^2]$), a quantity that provides information about whether the state is pure ($\mathcal{P}_Q = 1$) or mixed ($\mathcal{P}_Q < 1$), can be calculated analytically. In the present model, quantum purity can be calculated using Bessel properties [44–46]

$$
\begin{aligned}
\mathcal{P}_Q(t) = \text{Tr}[\rho(t)^2] &= \sum_{s_1=-\infty}^{\infty} \sum_{s_3=-\infty}^{\infty} \langle s_1|\rho(t)|s_3\rangle\langle s_3|\rho(t)|s_1\rangle \\
&= i^{(s_1-s_3)} e^{-2Dt} \sum_{n=-\infty}^{\infty} J_{s_1+n}\left(\frac{\Omega t}{\hbar}\right) J_{s_3+n}\left(\frac{\Omega t}{\hbar}\right) I_n(2Dt) \\
&\quad \times i^{(s_3-s_1)} e^{-2Dt} \sum_{n'=-\infty}^{\infty} J_{s_3+n'}\left(\frac{\Omega t}{\hbar}\right) J_{s_1+n'}\left(\frac{\Omega t}{\hbar}\right) I_{n'}(2Dt).
\end{aligned}
$$

Using the relations $\sum_{n=-\infty}^{\infty} J_{n+m}(x)J_{n+m'}(x) = \delta_{m,m'}$ and $\sum_{n=-\infty}^{\infty} I_n^2(x) = I_0(2x)$, we obtain
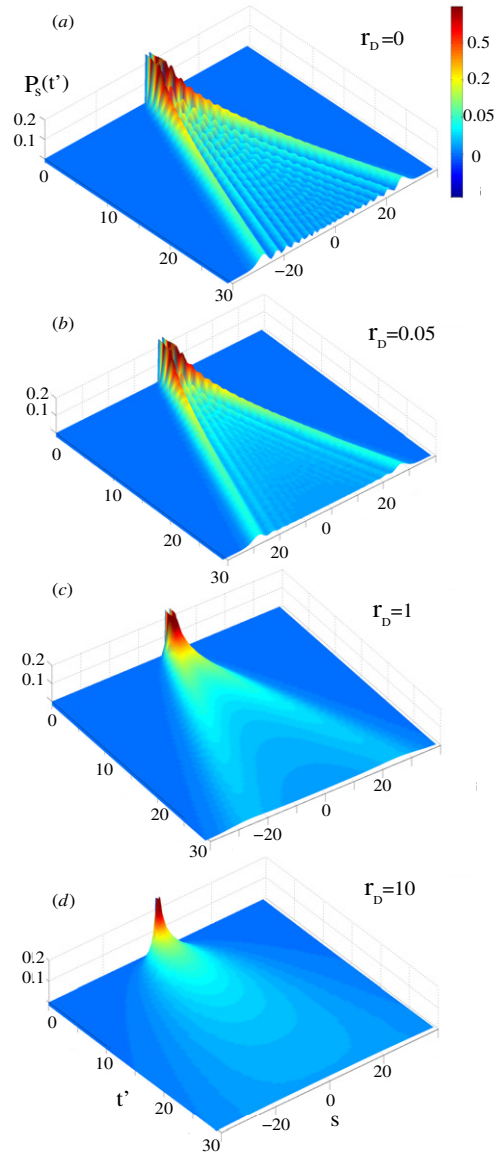
$$
\mathcal{P}_Q(t) = e^{-4Dt} I_0(4Dt).
$$

Figure 2. Representation in 3D of probability $P_s(t')$ for an initial condition $\rho(0) = |s_0\rangle\langle s_0|$ (where $s_0 = 0$) as a function of position s and t', for $r_D = 0, 0.05, 1, 10$ (*a*)–(*d*), where the blue regions indicate, approximately, value zero and red regions have high value for probability. The variables r_D and t' are the same as in figure 1.

The quantum purity takes the value one for $D = 0$ (without dissipation) for all time, and for the case $D \neq 0$ the quantum purity takes values smaller than one for $t > 0$ (mixed state). For $D \neq 0$, the quantum purity takes on the asymptotic power-law behavior $\mathcal{P}_Q(t) \sim t^{-1/2}$, for $t \to \infty$ (using $I_n(x) \approx \frac{e^x}{\sqrt{2\pi x}}$, for $x \to \infty$ [44]), in agreement with previous results presented in [41].

Another important measure that will indicate the presence of quantum behavior is the Wigner function. In the next subsection, we will study this function.

2.2. The Wigner function

The Wigner function was originally formulated as a quasi-probability for the position and momentum of the particle in quantum mechanics. For continuous variables X and K, representing position and momentum in the phase space, the Wigner function is given by [47, 48]

$$W(X, K, t) = \frac{1}{\pi} \int dY \langle X + Y | \rho(t) | X - Y \rangle e^{2iKY}, \tag{17}$$

where $\rho(t)$ is the time-dependent density operator. The Wigner function could have negative values whereby it is considered a quasi-joint probability of X and K, and the marginal distribution for X and K can be obtained in the usual form

$$\int dK W(X, K, t) = \langle X | \rho(t) | X \rangle, \tag{18a}$$

$$\int dX W(X, K, t) = \langle K | \rho(t) | K \rangle, \tag{18b}$$

where $\langle X | \rho(t) | X \rangle$ and $\langle K | \rho(t) | K \rangle$ are the time-dependent probability densities for X and K. The normalization condition for $\rho(t)$ can be checked from equation (17):

$$\int dX \int dK W(X, K, t) = \text{Tr}[\rho(t)] = 1. \tag{19}$$

In our DQW model, the space is an infinite one-dimensional regular lattice. Thus, in this case, we propose the Wigner function as

$$W(s, k, t) = \frac{1}{2\pi} \sum_{s'=-\infty}^{\infty} \langle s + s' | \rho(t) | s - s' \rangle e^{iks'}, \tag{20}$$

where $|s\rangle$ is a Wannier basis. This definition fulfils the required conditions for the Wigner function, see equations (18) and (19), using $\sum_s$ instead of $\int dX$, where $k \in [-\pi, \pi]$ (first Brillouin zone).

Using equation (13) in equation (20), we can write the Wigner function as follows:

$$W(s, k, t) = \frac{e^{-2Dt}}{2\pi} \sum_{n,s'=-\infty}^{\infty} i^{2s'} e^{iks'} J_{s+s'+n}\left(\frac{\Omega t}{\hbar}\right) J_{s-s'+n}\left(\frac{\Omega t}{\hbar}\right) I_n(2Dt), \tag{21}$$

then, after some algebra and using Bessel's properties [44–46] ($\sum_{n=-\infty}^{\infty} e^{in\gamma} J_{n+m}(x) J_n(x) = J_m(2x \sin(\gamma/2)) e^{i\beta m}$, where $\beta = \pi/2 - \gamma/2$), we find

$$W(s, k, t) = \frac{e^{-2Dt}}{2\pi} \sum_{n=-\infty}^{\infty} J_{2s+2n}\left(2\frac{\Omega t}{\hbar} \sin\frac{k}{2}\right) I_n(2Dt). \tag{22}$$

Using equations (18a) and (18b) in equation (22), we recover the probability densities for position s and momentum k respectively (see, equations (14) and (9)).

Interestingly, the Wigner function has information about the transition from DQW to CRW. Analyzing the case $D = 0$ (without dissipation in the system), the Wigner function adopts the following form:

$$W(s, k, t)_{QW} = \frac{1}{2\pi} J_{2s}\left(2\frac{\Omega t}{\hbar} \sin\frac{k}{2}\right), \quad D = 0. \tag{23}$$

In the pure diffusive regime ($\Omega = 0$, i.e. the CRW), the Wigner function can be written as

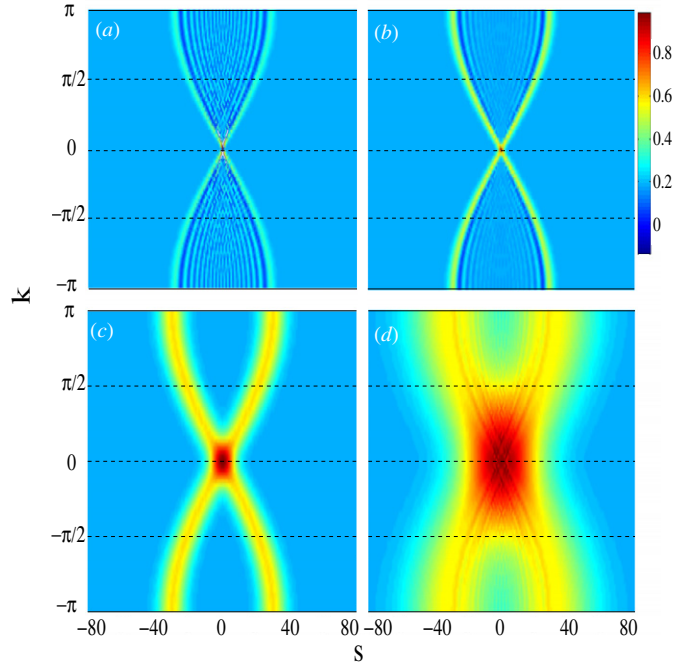$$W(s, k, t)_{CRW} = \frac{e^{-2Dt}}{2\pi} I_s(2Dt), \quad \Omega = 0. \tag{24}$$

9

Figure 3. Normalized Wigner function $W(s, k, t')/W_{max}$ as a function of position s and momentum k, for $r_D = 0$, 0.05, 1, 10 (a)–(d) and $t' = 30$, where W_{max} is the maximum value of Wigner function for each value of r_D. We have considered $r_D = \frac{2D}{\Omega/\hbar}$ and $t' = \frac{\Omega}{\hbar}t$ (dimensionless). The regions in blue indicate negative values, the ones in sky blue indicate, approximately, zero value and the red regions have the highest values of the Wigner function.

Then from equations (23) and (24), the Wigner function can be re-written as

$$W(s, k, t) = 2\pi \sum_{n=-\infty}^{\infty} W(s + n, k, t)_{QW}\, W(n, k, t)_{CRW}, \qquad (25)$$

then, changing $n \to -n$ and considering that $I_{-n}(x) = I_n(x)$, we obtain

$$W(s, k, t) = 2\pi \sum_{n=-\infty}^{\infty} W(s - n, k, t)_{QW}\, W(n, k, t)_{CRW}, \qquad (26)$$

this expression shows that the Wigner function of the DQW is given in terms of a non-trivial space convolution operation between the QW ($D = 0$) and the CRW ($\Omega = 0$). For the case $D \neq 0$, this expression shows the non-locality of the quantum mechanics of a free particle interacting with the quantum thermal $\mathcal{B}$.

In figure 3, we show the Wigner function from equation (22) or equation (26). We have normalized the Wigner function with respect to its maximum value W_{max} for each value of r_D (i.e. we use $W(s, k, t')/W_{max}$, where $t' = \frac{\Omega}{\hbar}t$ and $r_D = \frac{2D}{\Omega/\hbar}$). Similar Wigner's quantum carpets have been analyzed for a QW on a ring without dissipation in [49]. In figure 3(a), we observe the quantum behavior for $r_D = 0$. In this case the Wigner function has negative and positive values, and it shows remarkable oscillatory behavior (see equation (23)). In the case of small values of the dissipation, $r_D \ll 1$, we observe (figure 3(b), with $r_D = 0.05 \ll 1$) that the oscillatory behavior starts to diminish, and for values of $r_D \gtrsim 1$ (figures 3(c) and (d)) the dissipative term is dominant. In this case, the Wigner function takes only positive
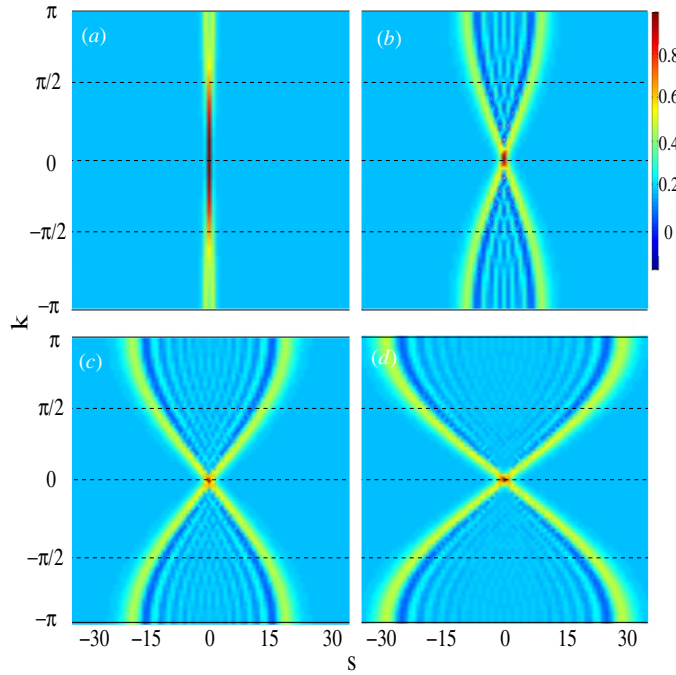
Figure 4. Normalized Wigner function $W(s, k, t')/W_{max}$ as a function of position s and momentum k, for $t' = 1, 10, 20, 30$ (a)–(d) and $r_D = 0.05$, in this case W_{max} is the maximum value of Wigner function for each value of t'.

values, therefore it is a well-defined joint probability, and the system resembles a CRW when r_D tends to infinity. In this case, the system is diffusive (see equation (24)).

In a complementary way, we now show the Wigner function (similar to figure 3), but we have fixed the parameter $r_D = 0.05$ and changed the dimensionless time t'. In figures 4(a)–(d), we observe the Wigner function for $t' = 1, 10, 20, 30$. The time evolution of the Wigner function also shows the transition from the DQW to the CRW.

In order to define a criterion to indicate when quantum correlations dominate over the classical correlations, or vice versa, we show in figure 5 the Wigner function $W_0 = W(0, \pi, t')$, as function of time t'. We note an oscillatory behavior of W_0 for $r_D < 1$. In the inset of figure 5, we show the Wigner function $W_1 = W(0, \pi, 1.9)$ as a function of r_D (we consider the value of t' where W_0 takes their first minimum). We use this as a criterion to indicate when quantum correlations are more important than classical correlations, and from figure 5, we note that for $r_D \lesssim r_D^c$, with $r_D^c = 0.52$, the Wigner function is $W_0 < 0$, therefore, the quantum correlations dominate in the system. For the case when $r_D > r_D^c$, the Wigner function is non-negative for all parameters in the system. In this case, the classical correlations dominate over the quantum correlations. Therefore, in this situation, we could say that the Wigner function is a joint probability density in the phase space (because $W(s, k, t) \geqslant 0$). This criterion is not unique, other criteria could also be used.

These results are consistent with the previous results obtained with the probability of finding the particle in the lattice site (see figures 1 and 2).
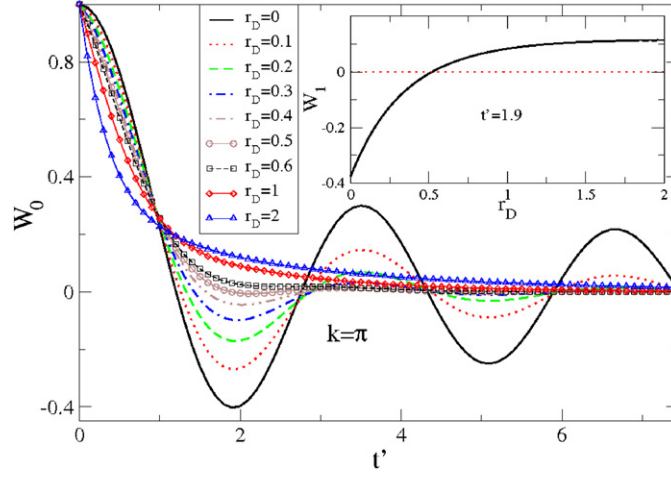
Figure 5. The Wigner function $W_0 = W(0, \pi, t')$ as a function of time t', for $r_D = 0, 0.1, 0.2,$ $0.3, 0.4, 0.5, 0.6, 1, 2$. The Wigner function $W_1 = W(0, \pi, 1.9)$, as a function of r_D, see inset. For $r_D \gtrsim 0.52$ the Wigner function is non-negative, and well defined as a joint probability density in the phase space.

2.3. The long-time limit of the reduced density matrix

In this subsection, we have analyzed the long-time limit behavior of the reduced density matrix. The equation (12) can be written in the form

$$\langle s_1 | \rho(t) | s_2 \rangle = \int_{-\pi}^{\pi} \frac{dk_1}{2\pi} e^{i \frac{\Omega t}{\hbar} \cos k_1} \mathcal{I}(k_1), \tag{27}$$

where

$$\mathcal{I}(k_1) = \int_{-\pi}^{\pi} \frac{dk_2}{2\pi} e^{-i \frac{\Omega t}{\hbar} \cos k_2} \cos\left[(k_1 - k_2)(s_1 - s_2)\right] e^{2Dt(\cos(k_1 - k_2) - 1)}. \tag{28}$$

By symmetry the term proportional to $\sin\left[(k_1 - k_2)(s_1 - s_2)\right]$ cancels out. Noting that in the long-time limit $\mathcal{I}(k_1)$ can be calculated by using the stationary phase approximation [50], we obtain (in the limit: $\Omega/\hbar \gg 2D$ and $t \to \infty$)

$$\mathcal{I}(k_1) \simeq \sqrt{\frac{2\pi \hbar}{\Omega t}} \left\{ e^{-2Dt(1 - \cos k_1) - i\left(\frac{\Omega t}{\hbar} - \pi/4\right)} \cos k_1 s_1 + e^{-2Dt(1 + \cos k_1) + i\left(\frac{\Omega t}{\hbar} - \pi/4\right)} \cos(k_1 s_1 - \pi s_2) \right\}.$$

Introducing this expression in equation (27) we can apply once again the stationary phase approximation (taking care that the saddle point $(0, 0)$ in the bi-dimensional integration does not contribute), then for the reduced density matrix in the asymptotic limit $((\Omega/\hbar)t \to \infty)$ we obtain

$$\langle s_1 | \rho(t) | s_2 \rangle \to \frac{2\hbar}{\pi \Omega t} \left\{ \cos \pi (s_1 + s_2) + \cos \pi (s_1 - s_2) \right.$$
$$+ e^{-4Dt} \left[\sin\left(2\frac{\Omega}{\hbar} t\right) \cos(s_1 + s_2)\frac{\pi}{2} \cos(s_1 - s_2)\frac{\pi}{2} \right]$$
$$\left. - i e^{-4Dt} \left[\cos\left(2\frac{\Omega}{\hbar} t\right) \sin(s_1 + s_2)\frac{\pi}{2} \sin(s_1 - s_2)\frac{\pi}{2} \right] \right\}. \tag{29}$$

This result is in agreement with the asymptotic approximation of the Bessel function when it is replaced in the equation (13) (for $x \to \infty$, $J_n(x) \approx \sqrt{\frac{2}{\pi x}} \cos(x - \frac{\pi}{4} - n\frac{\pi}{2})$). Thus, we see that for long time, terms proportional to e^{-4Dt} will contribute to the quantum entropy production associated with the reduced density matrix. In fact, this contribution is proportional to the following matrix (in Wannier representation):

$$
\begin{array}{c}
\cdots\cdots\cdots -1, \quad 0, \quad +1 \cdots\cdots\cdots\cdots \\
\end{array}
$$

$$
\begin{array}{c}
\vdots \\
\vdots \\
\vdots \\
-1 \\
0 \\
+1 \\
\vdots \\
\vdots \\
\vdots
\end{array}
\left(
\begin{array}{ccccccccc}
\ddots & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & A & -iB & A & -iB & A & -iB & A & \cdot \\
\cdot & iB & A & iB & A & iB & A & iB & \cdot \\
\cdot & A & -iB & A & -iB & A & -iB & A & \cdot \\
\cdot & iB & A & iB & A & iB & A & iB & \cdot \\
\cdot & A & -iB & A & -iB & A & -iB & A & \cdot \\
\cdot & iB & A & iB & A & iB & A & iB & \cdot \\
\cdot & A & -iB & A & -iB & A & -iB & A & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \ddots
\end{array}
\right),
\tag{30}
$$

where $A = \frac{2\hbar}{\pi \Omega t}(1 - \sin(2\Omega t/\hbar)e^{-4Dt})$, $B = \frac{2\hbar}{\pi \Omega t}\cos(2\Omega t/\hbar)e^{-4Dt}$. This means that asymptotically the probability profile $\rho_{ss}(t)$ goes to zero uniformly in the lattice, similar to $\sim \frac{2\hbar}{\pi \Omega t}(1 - \sin(2\Omega t/\hbar)e^{-4Dt}$, and the off-diagonal elements form a time-dependent coherent binary structure of $\{A, \pm iB\}$ (in the Wannier representation) that also goes to zero asymptotically as $\sim 1/t$. Due to the fact that Anderson's boundaries move at a finite velocity $V_A = \frac{1}{\sqrt{2}}\frac{\Omega}{\hbar}$ away from the initial condition (state $|s_0\rangle\langle s_0|$), we expect that the DQW will be always inside a (time-dependent) finite domain of maximum size $L \sim \sqrt{\langle \mathbf{q}(t)^2 \rangle - \langle \mathbf{q}(t)\rangle^2} \gg \epsilon$ (ϵ is the lattice parameter, we take $\epsilon = 1$), which increases linearly in time. Then, we can calculate the asymptotic eigenvalues of $\langle s_1| \rho(t) |s_2\rangle$ by approximating $\rho(t)$ to be a $L \times L$ finite-domain matrix.

It is simple to calculate the non-null eigenvalues of a matrix of dimension $L \times L$ of the form (30). For $D = 0$ (without dissipation) there is only one non-null eigenvalue:

$$
\lambda = \frac{2\hbar}{\pi \Omega t}\left[L - \sin\left(2\frac{\Omega}{\hbar}t\right)\right].
\tag{31}
$$

On the other hand, for the case $D \neq 0$, but $\Omega/\hbar \gg 2D$, we obtain only two non-null eigenvalues for the reduced density matrix. These eigenvalues are as follows:

$$
\lambda_\pm = \frac{2\hbar}{\pi \Omega t}\left\{ L - \sin\left(2\frac{\Omega}{\hbar}t\right) \right.
$$
$$
\left. \pm \sqrt{1 + (L^2 - 1)e^{-8Dt} - 2Le^{-4Dt}\sin\left(2\frac{\Omega}{\hbar}t\right) + e^{-8Dt}\sin^2\left(2\frac{\Omega}{\hbar}t\right)} \right\}.
\tag{32}
$$

As expected, we observe from this expression that if we take $D = 0$, we recover the equation (31). These results allow us to calculate the long-time behavior of the von Neumann entropy.

3. Quantum entanglement in the DQW

3.1. Time evolution of von Neumann's entropy

In order to study the irreversibility behavior of a free particle in interaction with a quantum thermal bath $\mathcal{B}$, i.e. our DQW model, we have calculated von Neumann's entropy corresponding to non-equilibrium situations, assuming that the system is prepared in a highly localized state (i.e. we adopt the initial condition $\rho(0) = |s_0\rangle \langle s_0|$, with $s_0 = 0$).

$$\mathcal{S}(t) = -\text{Tr}[\rho(t) \ln \rho(t)]. \tag{33}$$

In an open quantum system the reduced density matrix evolves in a Markovian approximation, following the QME (equation (2)). Due to the dissipation, the reduced density matrix $\rho(t)$ will not be diagonal at any time $t > 0$. The information of the quantum entanglement between the quantum thermal bath and our free particle—in the lattice—can be obtained from the reduced density matrix given in equation (13). Due to the fact that the total system is a pure state, the von Neumann entropy for the reduced density matrix can be used to measure the entanglement. Then we should calculate von Neumann's entropy numerically using $\rho(t)$ in the Wannier base. We have fixed the size of the chain to be L, with $L \approx V_A t$ where $V_A = \frac{1}{\sqrt{2}} \frac{\Omega}{\hbar}$, thus we have diagonalized the reduced density matrix. Then we can use the following expression for the quantum entropy:

$$\mathcal{S}(t) = -\sum_i \Lambda_i \ln \Lambda_i, \tag{34}$$

where Λ_i is an eigenvalue of the reduced density matrix $\langle s_1 | \rho(t) | s_2 \rangle$ in the domain $[-L, L]$. We expect that for finite times (even in an infinite lattice) $\mathcal{S}(t) \neq \infty$. We have carried out this calculation numerically and we have shown in figure 6 $\mathcal{S}(t)$ as a function of time $t' = \frac{\Omega}{\hbar} t$ for different values of the dissipative parameter $r_D = \frac{2D}{\Omega/\hbar}$.

In figure 6(a), we observe the quantum entropy as a function of r_D and t' (3D visualization). As expected for $r_D = 0$ ($D = 0$), the quantum entropy is $\mathcal{S}(t') = 0$ for all $t' \geqslant 0$. In this case the quantum entanglement between the free particle in the lattice and the phonon bath is zero, which means we can write the wavefunction of the total system as a product of one state of the free particle in the lattice and one of the phonon bath (separable state). Another trivial result is the case that $t' = 0$, where the quantum entropy is zero for $r_D \geqslant 0$ (in this case $\rho(t' = 0) = |s_0\rangle\langle s_0|$). In the presence of dissipation the total system is no longer a separable state between the particle in the lattice and environment. The reduced density matrix $\rho(t)$ is a mixed state (for $D > 0$), and the quantum entropy starts increasing in time for a fixed value of r_D. We also note that for a fixed value of t', the magnitude of the quantum entropy increases as r_D increases. The quantum entropy gives information about the transition from the DQW to the CRW, which is consistent with the results obtained above concerning the probability profile and the Wigner function. Finally, in figure 6(b), we show results of the quantum entropy as a function of t' and different values of r_D.

Similar analyses to measure quantum correlations have been carried out by considering a free particle (in a lattice) with an additional internal degree of freedom: the quantum 'coin'. Thus, the correlation between the *coin* and the *spatial* degree of freedom has been studied in detail, and these models share some similarities with our results despite the fact that by considering *the quantum coin* as the thermal bath, the latter has a finite Hilbert space [17, 51].

Interestingly, by introducing the stationary phase approximation in equation (12), it is possible to obtain asymptotic behavior for $\langle s_2 | \rho(t) | s_1 \rangle$, then we can study the time dependence of $\mathcal{S}(t)$ in the long-time regime analytically.
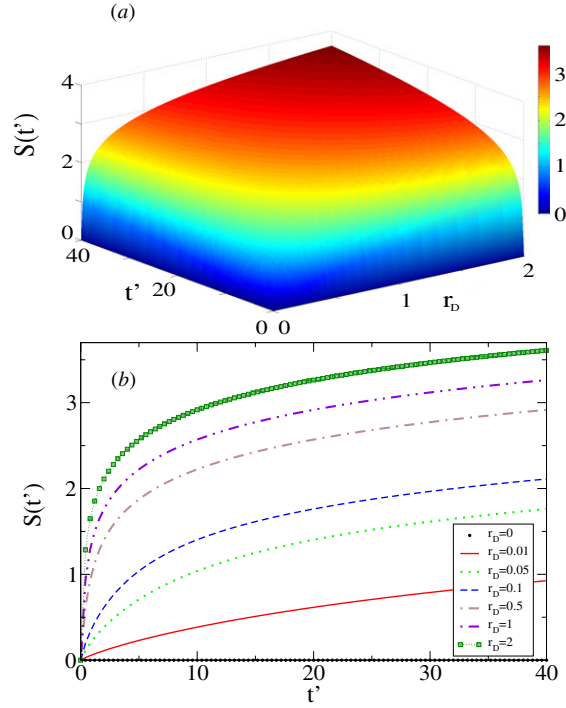
Figure 6. von Neumann's entropy as a function of t' and r_D (a). This function measures the quantum entanglement between the particle in the lattice and the phonons bath. We show a plot in 2D (b) of quantum entropy as a function of t' for different values of $r_D = 0, 0.01, 0.05, 0.1, 0.5, 1, 2$.

3.1.1. The long-time limit of von Neumann's entropy. Having the result of equation (29) we can re-write von Neumann's entropy in the long-time regime in the form

$$\mathcal{S}(t) = -\sum_{s_1=-\infty}^{\infty} \sum_{s_2=-\infty}^{\infty} \langle s_1 | \rho(t) | s_2 \rangle \langle s_2 | \ln \rho(t) | s_1 \rangle$$

$$\simeq -\sum_{j=1}^{L} \lambda_j \ln \lambda_j, \tag{35}$$

here λ_j are the eigenvalues associated with the asymptotic long-time regime of the reduced density matrix $\langle s_1 | \rho(t) | s_2 \rangle$. Using equation (32) in equation (35) and considering $L \gg 1$ (for simplicity, we re-normalized the eigenvalues of $\rho(t)$), we obtain (when $\frac{\Omega}{\hbar} \gg 2D$ and $\frac{\Omega}{\hbar} t \gg 1$)

$$\mathcal{S}(t) \simeq -\left(\frac{1 - e^{-4Dt}}{2}\right) \ln\left(\frac{1 - e^{-4Dt}}{2}\right) - \left(\frac{1 + e^{-4Dt}}{2}\right) \ln\left(\frac{1 + e^{-4Dt}}{2}\right). \tag{36}$$

In addition, another asymptotic approximation to $\mathcal{S}(t)$ can be made if we consider $D \sim 0$ (with $Dt \ll 1$), so we can approximate $e^{-4Dt} \to 1 - 4Dt$ and replacing this expression in equation (36) we get a simpler expression for the quantum entropy in the form

$$\mathcal{S}(t) \simeq -2Dt \ln(2Dt), \quad Dt \ll 1.$$

15

Note that in the limit $D \to 0$ (even when $t \gg 1$) the quantum entropy $\mathcal{S}(t) \to 0$. We have checked this analytical result with our numerical calculation using equation (34) and the agreement is excellent, see figure 6.

4. Conclusions

A free particle—in an infinite regular lattice—in interaction with a thermal phonon bath has been studied by tracing out the degree of freedom of the bath. We then worked out the quantum master equation for a dissipative tight-binding model.

   We have solved the master equation analytically by using Bessel functions, and obtained the reduced density matrix $\rho(t)$ as a function of the scale energies of the system ($\Omega/\hbar$, D). We have also studied the transition from dissipative quantum walk (DQW) to classical random walk (CRW) in terms of parameters D and $\Omega/\hbar$ (or $r_D = \frac{2D}{\Omega/\hbar}$). In the case when $2D \ll \Omega/\hbar$ ($r_D \ll 1$), the quantum behavior is more important than the dissipation in the system. In the opposite case, we re-obtain the CRW $2D \gg \Omega/\hbar$ ($r_D \gg 1$) because in this case the dissipation creates decoherence in the system. We have studied the Wigner function to analyze the pseudo-probability densities in the phase space. This function is very useful as an indicator of this quantum–classical transition.

   As an alternative approach to the study of the transition from DQW to CRW we have used tools from quantum information theory (as a function of dissipative parameter) to analyze the reduced density matrix. To describe this transition we have used von Neumann's entropy $\mathcal{S}(t)$ to measure the quantum entanglement between the free particle—in a lattice—and the phonon bath. We observed that for $D = 0$ the quantum entropy is $\mathcal{S}(t') = 0$ for $t' \geqslant 0$ (closed system), and when D increases we show that quantum decoherence starts to appear and therefore the quantum entropy increases in time with a law which is slower than that from classical statistics ($\mathcal{S}(t)_{CRW} \sim \ln t$) [6, 28]. Asymptotically for $D \to 0$, the quantum entropy turns out to be only a function of the dissipative parameter D. This fact also indicates the beginning of the transition from the DQW to the CRW.

   This analytical model allows us to study the effect of decoherence in the DQW as a function of the two typical energies of the system. We can conclude that in the present this model there are two characteristic time scales: the dissipative time $\tau_D \sim 1/D$ and the hopping time $\tau_H \sim \hbar/\Omega$; the competition between these time scales controls the decoherence and correlation mechanism in the system. For example, the quantum purity $\mathcal{P}_Q(t)$ is controlled by τ_D, but in general the entropy and the interference phenomena appearing in the probability profile or in the Wigner phase space pseudo-distribution are controlled by the competition between these time scales.

   The interesting problem of the propagation of photons in waveguide lattices is possible scenarios where our present results can be applied, also the analysis of the entanglement of a bipartite system can be studied in the present framework, works along these lines are in progress. In this way, the present model gives insight into the effect of dissipation in more complex quantum systems, for instance, the analysis of quantum correlations between two particles—in a regular lattice—in interaction with a phonon bath.

Acknowledgments

Appendix A. On the second quantization and the one-particle tight-binding Hamiltonian

A free Hamiltonian in the tight-binding approximation for spinless particles (fermion) can be written in second quantization in the form [52]

$$H_S = E_0 \sum_{s=-\infty}^{\infty} c_s^\dagger c_s - \frac{\Omega}{2} \left(\sum_{s=-\infty}^{\infty} c_{s-1}^\dagger c_s + c_{s+1}^\dagger c_s \right), \tag{A.1}$$

where $c_s^\dagger$ and c_s are creation and destruction operators in the site s of the lattice respectively $(|\ldots, 0, 1_s, 0, \ldots\rangle = c_s^\dagger |0\rangle$, where $|0\rangle$ is the empty state). Then considering only one particle it is straightforward to compare equation (A.1) with H_S in equation (1), if we replace a and $a^\dagger$ with a combination of $c_{s'}^\dagger$ and $c_{s'}$, in the following way:

$$a \Rightarrow R = \sum_{s=-\infty}^{\infty} c_{s-1}^\dagger c_s, \quad a^\dagger \Rightarrow R^\dagger = \sum_{s=-\infty}^{\infty} c_{s+1}^\dagger c_s, \tag{A.2}$$

where c_s are acting in the Fock space. Therefore, we can also check that R and $R^\dagger$ commute in the general case for many particles (where $R^\dagger R = RR^\dagger = \sum_{s=-\infty}^{\infty} c_s^\dagger c_s - \sum_{s,s'=-\infty}^{\infty} c_{s+1}^\dagger c_{s'-1}^\dagger c_s c_{s'}$), and for one particle in the lattice we obtain $RR^\dagger = \mathbf{1}$.

Equation (A.2) shows the expected mapping from Fock's space into the Winner basis. Then the connection between the tight-binding Hamiltonian and the QW model can be established.

Appendix B. Reduced matrix density

Here, we show how to obtain equation (13). Replacing the following relations for the Bessel function $e^{iz\cos\theta} = \sum_{n=-\infty}^{\infty} i^n J_n(z) e^{in\theta}$; $e^{z\cos\theta} = \sum_{n=-\infty}^{\infty} I_n(z) e^{in\theta}$ in equation (12), where J_n and I_n are a Bessel functions of integer order [44, 45], we find

$$\langle s_1 | \rho(t) | s_2 \rangle = \left(\frac{1}{2\pi} \right)^2 e^{-2Dt} \sum_{m_1, m_2, n=-\infty}^{\infty} J_{m_1} \left(\frac{\Omega t}{\hbar} \right) J_{m_2} \left(\frac{\Omega t}{\hbar} \right) I_n(2Dt)$$

$$\times i^{m_1+m_2} \int_{-\pi}^{\pi} dk_1 e^{i(s_1+m_2+n)k_1} \int_{-\pi}^{\pi} dk_2 e^{-i(s_2-m_1+n)k_2}.$$

Using the definition of Kronecker delta: $\delta_{s,s'} = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{ik(s-s')}$ in the previous expression, we finally obtain

$$\langle s_1 | \rho(t) | s_2 \rangle = i^{(s_1-s_2)} e^{-2Dt} \sum_{n=-\infty}^{\infty} J_{s_1+n} \left(\frac{\Omega t}{\hbar} \right) J_{s_2+n} \left(\frac{\Omega t}{\hbar} \right) I_n(2Dt).$$

Appendix C. Moments of the position operator—the characteristic function

We have defined a characteristic function [6] for calculating moments of position operator $\mathbf{q}$ in the following way:

$$\mathcal{G}(\xi) = \mathrm{Tr}[\rho(t) e^{i\xi \mathbf{q}}] = \sum_{l=-\infty}^{\infty} \langle l | \rho(t) | l \rangle e^{i\xi l}, \tag{C.1}$$

thus the quantum moments of **q** can be obtained using the following expression:

$$\langle \mathbf{q}(t)^m \rangle = \frac{1}{i^m} \frac{\mathrm{d}^m}{\mathrm{d}\xi^m} \mathcal{G}(\xi) \bigg|_{\xi=0}, \tag{C.2}$$

Using equation (13) in equation (C.1), we can write the characteristic function in the form

$$\mathcal{G}(\xi) = \mathrm{e}^{-2Dt(1-\cos\xi)} J_0 \left(2t \frac{\Omega}{\hbar} \sin \frac{\xi}{2} \right), \tag{C.3}$$

here we have said that $\sum_{n=-\infty}^{\infty} \mathrm{e}^{in\gamma} J_{n+m}(x) J_n(x) = J_m(2x \sin(\gamma/2)) \, \mathrm{e}^{i\beta m}$, where $\beta = \pi/2 - \gamma/2$. From this characteristic function all the moments of the position operator can be calculated straightforwardly. In particular, we can re-obtain the variance of the DQW (see equation (7)). Note that in the classical limit $\Omega = 0$ we recover the expected characteristic function associated with the CRW [6, 28]. In general, equation (C.3) shows that the non-equilibrium behavior of the characteristic function of the DQW is the product of the classical one and the quantum characteristic function $J_0 \left(2t \frac{\Omega}{\hbar} \sin \frac{\xi}{2} \right)$.

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