Quantum Random Walks and Piecewise Deterministic Evolutions

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In the continuous space and time limit, we show that the probability density to find the quantum random walk (QRW) driven by the Hadamard "coin" solves a hyperbolic evolution equation similar to the one obtained for a random two-velocity evolution with spatially inhomogeneous transition rates between the velocity states. In spite of the presence of a nonlinear drift term, it is remarkable that the QRW position can easily be described in simple analytical terms. This allows us to derive the quadratic time dependence of the variance typical for the QRW.

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In the last ten years a sustained attention has been devoted to the study of quantum random walks (QRW) on graphs and lattices and a recent introductory survey is given in the paper by Kempe [1]. The term QRW was coined in 1993 in [2]. QRW are systems analogous to classical random walks but exhibit a radically different behavior. Consider the simplest situation, namely, a discrete time walk on the one dimensional lattice $\mathbb{Z}$. The QRW possesses an extra coin degree of freedom. Exactly as in the classical random walk the direction that the walker moves is determined by the outcome of a coin flip. In the case of a quantum walk the flip of the coin as well as the conditional motion of the walker are both given by unitary transformations, making therefore possible interferences of paths. For the classical walk the probability $P(n, \tau)$ to find the particle at time τ in $n \in \mathbb{Z}$ is a binomial distribution with a variance σ^2 growing linearly with time, so the expected distance from the origin is of the order $\sigma \sim \tau^{1/2}$. By contrast and due to the presence of interferences, the variance of the QRW scales as $\sigma^2 \sim \tau^2$, from which it follows that the expected distance from the origin is of the order $\sigma \sim \tau$. In other words the quantum random walk propagates quadratically faster as the classical one. The unitary transformation C describing the coin flip in the two dimensional coin space $\mathcal{H}$ is frequently given by the Hadamard transformation H:

$$H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \tag{1}$$

The total Hilbert space $\mathcal{H}$ describing the position and the coin dynamics is in this simple situation nothing else as the tensor product taking into account the 2 degrees of freedom, space and spin,

$$\mathcal{H} = \ell^2 \otimes \mathbf{C}^2,$$

and the conditional space translation of the particle is given by a unitary operator S and depends on its spin degree of freedom.

Let us briefly recall [2,3] that to describe the motion QRW, one usually introduces a spinlike degree of freedom (i.e., often called the *chirality*) which can take the values Left and Right or a superposition. One then considers a two-component wave function:

$$\begin{pmatrix} \psi_L(n, \tau) \\ \psi_R(n, \tau) \end{pmatrix}$$

characterizing the amplitudes of the QRW to be at $n \in \mathbb{Z}$ at time τ. The 1D QRW is then defined to be the motion of a test particle on the lattice $\mathbb{Z}$ which at each time step suffers a modification of its chirality according to the rule induced by Eq. (1) and then the particle moves to its (new) chirality state given by a superposition of positions:

$$\psi_L(n, \tau + 1) = -\frac{1}{\sqrt{2}}\psi_L(n + 1, \tau) + \frac{1}{\sqrt{2}}\psi_R(n - 1, \tau),$$

$$\psi_R(n, \tau + 1) = \frac{1}{\sqrt{2}}\psi_L(n + 1, \tau) + \frac{1}{\sqrt{2}}\psi_R(n - 1, \tau), \tag{2}$$

with $n \in \mathbb{Z}$. As pointed out in [3], the above relations are both equivalent to

$$a(n, \tau + 1) - a(n, \tau - 1) = \frac{1}{\sqrt{2}}[a(n - 1, \tau) - a(n + 1, \tau)] \tag{3}$$

with either $a(n, \tau) = \psi_L(n, \tau)$ or $a(n, \tau) = \psi_R(n, \tau)$. To explicitly restore the dual role played by the ψ_R and the ψ_L in Eq. (2), we further introduce

$$a(n, \tau) = A^+(n, \tau) + (-1)^\tau A^-(n, \tau), \tag{4}$$

in terms of which Eq. (2) reads

$$A^{\pm}(n, \tau + 1) - A^{\pm}(n, \tau - 1) = \pm \frac{1}{\sqrt{2}}[A^{\pm}(n-1, \tau) - A^{\pm}(n+1, \tau)]. \quad (5)$$

We can now rewrite Eq. (5) as a second order recurrence, namely,

$$\mathbb{T}(\tau)A^{+}(n, \tau) = \frac{1}{\sqrt{2}}\Delta(n)A^{+}(n, \tau) - \sqrt{2}[A^{+}(n+1, \tau) - A^{+}(n, \tau)] \quad (6)$$

and

$$\mathbb{T}(\tau)A^{-}(n, \tau) = \frac{1}{\sqrt{2}}\Delta(n)A^{-}(n, \tau) + \sqrt{2}[A^{-}(n, \tau) - A^{-}(n-1, \tau)], \quad (7)$$

where the two-step difference operators are defined as

$$\mathbb{T}(\tau)A^{\pm}(n, \tau) = A^{\pm}(n, \tau+1) - 2A^{\pm}(n, \tau) + A^{\pm}(n, \tau-1) + 2[A^{\pm}(n, \tau) - A^{\pm}(n, \tau-1)]$$

and

$$\Delta(n)A^{\pm}(n, \tau) = A^{\pm}(n+1, \tau) - 2A^{\pm}(n, \tau) + A^{\pm}(n-1, \tau).$$

Except at the origin $n = 0$, the continuous limit of Eqs. (6) and (7) can be written unambiguously in terms of the continuous variables $\tau \mapsto t \in \mathbb{R}^{+}$ and $n \mapsto x \in \mathbb{R}$ as

$$\frac{\partial^2}{\partial t^2}A^{\pm}(x, t) + 2\frac{\partial}{\partial t}A^{\pm}(x, t) = \sqrt{2}\left[\frac{1}{2}\frac{\partial^2}{\partial x^2}A^{\pm}(x, t) \pm \frac{\partial}{\partial x}A^{\pm}(x, t)\right]. \quad (8)$$

The hyperbolic equation (8) is the Chapman-Kolmogorov equation for probability densities governing piecewise deterministic evolution models [4]. When time $t \to \infty$ the densities $A^{\pm}(x, t)$ will reach a diffusive regime [4,5] characterized by a left, respectively, a right drifted Gaussian:

$$A^{\pm}(x, t) \simeq \mathcal{N} e^{-(x \pm \sqrt{2}t)^2/2\sqrt{2}\,t} \quad \text{for } t \to \infty, \quad (9)$$

with $\mathcal{N}$ a normalization factor. Returning to the original QRW, the probability $P(n, \tau)$ to find the walker at position n at the (discrete) time τ is given by

$$P(n, \tau) \simeq [p_1 A^{+}(n, \tau) + (-1)^{\tau} p_2 A^{-}(n, \tau)]^2 \qquad \tau \in \mathbb{N}, \quad (10)$$

where p_1 and p_2 are two constants determined by the initial condition and the normalization constraint. In the following the calculations will be performed with $p_1 = p_2$ which corresponds to a symmetric initial condition $P(n, 0) = \delta_{n,0}$. Note however that we can proceed along the same lines for $p_1 \neq p_2$. The rapid and bounded oscillations induced by the $(-1)^{\tau}$ contributions in Eq. (10) will be smeared out in the large time limit. Hence for asymptotically large times, we can write

$$P(n, \tau) \simeq [A^{+}(n, \tau)]^2 + [A^{-}(n, \tau)]^2 \qquad \tau \gg 1. \quad (11)$$

In view of Eq. (9), the time and space continuous limit of Eq. (11) can be now written as

$$P(x, t) \simeq \mathcal{N}' e^{-\sqrt{2}t} \cosh(2x) e^{-x^2/\sqrt{2}t} \quad \text{for } t \to \infty. \quad (12)$$

It is known [6,7] that Eq. (12) solves itself as a (diffusive) Fokker-Planck equation with a nonlinear drift. Indeed, introducing the rescaled variables $s \mapsto 2\sqrt{2}t$ and $y = 2x$, it is immediate to see that Eq. (12) solves

$$\frac{\partial}{\partial s}P(y, s) = \frac{1}{2}\frac{\partial^2}{\partial y^2}P(y, s) - \frac{\partial}{\partial y}[\tanh(y)P(y, s)]. \quad (13)$$

Note that the probability density given by Eq. (12) exhibits a transition from a unimodal to a bimodal shape at the time $t_c = 2\sqrt{2}t$, a behavior typical for the QRW.

Clearly Eq. (13) is a parabolic partial differential equation whereas the original models given by Eqs. (6) and (7) are basically hyperbolic time evolutions (i.e., they involve a second order recurrence in time). To restore the hyperbolic character in the continuous limit, we observe that Eq. (13) itself describes the diffusive regime of the probability density $P_h(y, s)$ governing a random two-velocity model of the Kac's type [8] with spatially inhomogeneous transition rates between the velocities. This class of random evolutions is discussed in [4]. For this two-velocity model, the equation for the transition probability reads

$$\frac{1}{2\beta^2}\frac{\partial^2}{\partial s^2}P_h(y, s) + \frac{\partial}{\partial s}P_h(y, s) = \frac{1}{2}\frac{\partial^2}{\partial y^2}P_h(y, s) - \frac{\partial}{\partial y}[\tanh(y)P_h(y, s)]. \quad (14)$$

As explained in [4], the parameter $\beta > 1$ is the rate of change between the two-velocity states of the random evolution. The solution of Eq. (14) follows directly if one introduces the transformation:

$$P_h(y, s) = e^{-\beta^2 s}\cosh(y)Q(y, s). \quad (15)$$

In terms of $Q(y, s)$ Eq. (14) reads

$$\frac{1}{\beta^2}\frac{\partial^2}{\partial s^2}Q(y,s) - \frac{\partial^2}{\partial y^2}Q(y,s) + (1-\beta^2)Q(y,s) = 0. \tag{16}$$

From now on, we shall adopt the notation:

$$u = \beta s \quad \text{and} \quad \gamma = \sqrt{\beta^2 - 1} \in \mathbb{R}^+.$$

For the initial conditions $P_h(y,0) = A(y)$, respectively, $\dot{P}_h(y,0)B(y)$ which, in view of Eq. (15) implies $\cosh(y)\,Q(y,0) = A(y)$, respectively, $\cosh(y) \times \dot{Q}(y,u)|_{u=0} = \beta^2 A(y) + B(y)$, the final solution reads as [5,9]

$$P_h(y,s) = \frac{\cosh(y)}{2}e^{-\beta u}\left\{\left[\frac{A(y+u)}{\cosh(y+u)} + \frac{A(y-u)}{\cosh(y-u)}\right] + \Gamma_1(y,u) + \Gamma_2(y,u)\right\}, \tag{17}$$

with Γ_1 and Γ_2 given by

$$\Gamma_1(y,u) = \int_{y-u}^{y+u} I_0[\gamma\sqrt{u^2-(y-z)^2}]\frac{\beta^2 A(z) + B(z)}{\cosh(z)}dz$$

and

$$\Gamma_2(y,u) = \gamma u \int_{y-u}^{y+u} \frac{I_1[\gamma\sqrt{u^2-(y-z)^2}]}{\sqrt{u^2-(y-z)^2}}\frac{A(z)}{\cosh(z)}dz,$$

where $I_\nu(x)$ stands for the modified Bessel function of integer order ν. Let us study the behavior of the solution given by Eq. (17) as a function of s. We consider symmetric walks, characterized by

$$P_h(y,0) = \delta(y) \quad \text{and} \quad \dot{P}_h(y,0) = 0 \tag{18}$$

which, in view of Eq. (17) with $A(y) = \delta(y)$ and $B(y) = 0$, implies (for the probability density)

$$P_h(y,u) = e^{-\beta u}\frac{\cosh(y)}{2} \times \{[\delta(y-u) + \delta(y+u)] + \psi(y,u)\} \times \Theta(|\,y\,| - u), \tag{19}$$

with

$$\psi(y,u) := \beta^2 I_0[\gamma\sqrt{u^2-y^2}] + \gamma u \frac{I_1[\gamma\sqrt{u^2-y^2}]}{\sqrt{u^2-y^2}}, \tag{20}$$

and $\Theta(x)$ is 1 for positive x and 0 otherwise. Clearly, the solution given by Eq. (19) has a compact support and exhibits two propagating point measures, [i.e., $\delta(y \pm u)$ located on the characteristics of the hyperbolic evolution Eq. (14)]. In addition, a bimodal shape of $P_h(y,u)$ arises at the critical time u^* defined by the sign change of the curvature $\mathcal{R}(u)$ at $y = 0$. We, namely, have

$$\mathcal{R}(u^*) = \frac{\partial^2}{\partial y^2}P_h(y,u^*)|_{y=0} = 0. \tag{21}$$

A direct calculation yields

$$\mathcal{R}(u) := \frac{\partial^2}{\partial y^2}P_h(y,u)|_{y=0} = \frac{e^{-\beta u}}{2}\left\{\beta^2 I_0(\gamma u) + \gamma I_1(\gamma u) - \frac{1}{\gamma u}[\beta^2 I_1(\gamma u) + \gamma I_2(\gamma u)]\right\}. \tag{22}$$

The curvature $\mathcal{R}(u)$ given by Eq. (22) behaves as $\lim_{u\to 0}\mathcal{R}(u) < 0$ and conversely, using the fact that $I_\nu(y) \simeq (e^y/\sqrt{2\pi y})$ for $y \to \infty$, we have $\lim_{u\to\infty}\mathcal{R}(u) > 0$. This behavior together with the symmetry of $P_h(y,u)$ indicates a transition from a unimodal to a bimodal shape for $P_h(y,u)$. Note that $P_h(y,u)$ can only be bimodal as it is the product of a $\cosh(y)$ with the concave symmetric function $\psi(y,u)$ given in Eq. (20). This bimodal character of the probability density is typical for the symmetric QRW [1,3]. Finally, the variance $\sigma^2_{\mathrm{QRW}}(u)$ of the QRW reads as

$$\sigma^2_{\mathrm{QRW}}(u) = \int_{-\infty}^{+\infty} P_h(y,u)y^2 dy. \tag{23}$$

For $u \to \infty$ we are in the diffusive regime and we can use Eq. (12) to approximately write

$$\sigma^2_{\mathrm{QRW}}(u) \simeq \frac{e^{-(u/2\beta)}\sqrt{\beta}}{\sqrt{2\pi u}}\int_{-\infty}^{+\infty}\cosh(y)e^{-(\beta y^2/2u)}y^2 dy = \left(\frac{u}{\beta}\right)^2 + \frac{u}{\beta}. \tag{24}$$

This quadratic dependence characterizes the behavior expected for the QRW [1].

It is important to emphasize that while only the Hadamard coin was here used to derive Eq. (14), the general class of unitary evolutions for the spin will lead to a general class of hyperbolic equations describing piecewise deterministic motions. Note however that the dynamics induced by the Hadamard coin offers a great analytical simplicity which is due to the fact that the Sturm-Liouville problem arising when solving Eq. (14) is in this case trivial.

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