Convergence of continuous-time quantum walks on the line

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Abstract

The position density of a "particle" performing a continuous-time quantum walk on the integer lattice, viewed on length scales inversely proportional to the time t, converges (as t tends to infinity) to a probability distribution that depends on the initial state of the particle. This convergence behavior has recently been demonstrated for the simplest continuous-time random walk [1]. In this brief report, we use a different technique to establish the same convergence for a very large class of continuous-time quantum walks, and we identify the limit distribution in the general case.

An article recently published in this journal [1] proves that a certain "continuous-time quantum walk" on the integer lattice $\mathbb{Z}$ has the same kind of convergence behavior as "coined quantum walks" on $\mathbb{Z}$ have [2, 3]. In this note, the convergence result of [1] is generalized to a large class of continuous-time quantum walks, using the techniques developed in [4, 5] for coined quantum walks. An interesting aspect of the generalized continuous-time quantum walk is that the limiting measure need not have compact support.

Continuous time quantum walks on graphs were first defined in [6] as follows. Consider a graph with vertex set V. Let L_γ denote the infinitesimal generator of the continuous-time Markov jump process on V, where jumps only occur between adjacent vertices and the jumping rates are all equal to some $\gamma > 0$. The continuous-time quantum walk of [6] amounts to the unitary dynamics

$$\psi_0 \;\longmapsto\; e^{-itL_\gamma}\psi_0 \tag{1}$$

on $\ell^2(V)$, the Hilbert space of square-summable complex-valued functions on V. Other authors [7, 8] have defined continuous-time quantum walk as the dynamics

$$\psi_0 \;\longmapsto\; e^{-itA}\psi_0 \;, \tag{2}$$

using the operator defined by the adjacency matrix A of the graph instead of L_γ. When the graph is the integer lattice $\mathbb{Z}$, it hardly matters which way the continuous-time quantum walk is defined, for $L_\gamma = (1-2\gamma)I + \gamma A$ and therefore (1) and (2) differ only by a change of time and phase.

In [1], Norio Konno studies the continuous-time quantum walk on $\mathbb{Z}$ defined as in (2) but with $-t/2$ instead of t. That is, he studies the dynamics $\psi_0 \mapsto e^{i(t/2)A}\psi_0$, where A denotes the operator on $\ell^2(\mathbb{Z})$ whose matrix with respect to the standard orthonormal basis $\{e_n\}$ is the adjacency matrix for the integer lattice (the standard basis vector e_n is the member of $\ell^2(\mathbb{Z})$ with $e_n(n) = 1$ and $e_n(k) = 0$ for all $k \neq n$). In this case the operators $e^{i(t/2)A}$ can be expressed exactly in terms of Bessel functions, and the following convergence behavior becomes evident [1]: For each t, define the probability measures

$$P_t(n) \;=\; \left|\langle e_n, e^{i(t/2)A}e_0\rangle\right|^2$$

on $\mathbb{Z}$. Then

$$\lim_{t\to\infty} \sum_{at\le k\le bt} P_t(k) \;=\; \int_a^b \frac{dx}{\pi\sqrt{1-x^2}}$$

for $-1 \le a < b \le 1$.

This result is a special case of a much more general proposition. The main condition is that the generator A of the quantum walk (2) be a self-adjoint operator that commutes with translations of $\ell^2(\mathbb{Z})$. Any such A has a matrix representation (with respect to the standard basis) of the form

$$\begin{bmatrix} \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \\ \ddots & a_0 & \overline{a_1} & \overline{a_2} & \overline{a_3} & \ddots & \ddots \\ \ddots & a_1 & a_0 & \overline{a_1} & \overline{a_2} & \overline{a_3} & \ddots \\ \ddots & a_2 & a_1 & a_0 & \overline{a_1} & \overline{a_2} & \ddots \\ \ddots & a_3 & a_2 & a_1 & a_0 & \overline{a_1} & \ddots \\ \ddots & \ddots & a_3 & a_2 & a_1 & a_0 & \ddots \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \end{bmatrix} \tag{3}$$

with $a_0 = \overline{a_0}$. We will only consider self-adjoint operators A that are Fourier transforms of a multiplication operator, in the following sense. We denote the circle of unit radius by $\mathbb{T}$ and parameterize it by $0 \le \theta < 2\pi$. $L^2(\mathbb{T}, \frac{d\theta}{2\pi})$ denotes the Hilbert space of square-integrable functions $\mathbb{T}$. The Fourier transform

$$(\mathcal{F}f)(n) \;=\; \int_{\mathbb{T}} f(\theta) e^{-in\theta}\, \tfrac{d\theta}{2\pi}$$

is a unitary isomorphism from $L^2(\mathbb{T}, \frac{d\theta}{2\pi})$ to $\ell^2(\mathbb{Z})$ with inverse

$$(\mathcal{F}^*\psi)(\theta) \;=\; \sum_{n\in\mathbb{Z}} \psi(n) e^{in\theta}\;.$$

We will assume that there exists a measurable real-valued function $\widehat{a}(\theta)$ on $\mathbb{T}$ such that A satisfies $(\mathcal{F}^* A \mathcal{F} f)(\theta) = \widehat{a}(\theta) f(\theta)$ whenever f and $\widehat{a}f$ are both in $L^2(\mathbb{T}, \frac{d\theta}{2\pi})$. We will further assume that $\widehat{a}(\theta)$ is differentiable at almost every $\theta \in \mathbb{T}$. These assumptions on the form of A permit us vastly to generalize the main result of [1] fairly easily, but they are rather technical. Perhaps a more convenient (but less general) condition is that the entries of the matrix (3) satisfy $\sum_{n=1}^{\infty} n|a_n| < \infty$, for this implies that A has the desired form with $\widehat{a}(\theta) = a_0 + \sum_{n=1}^{\infty} (a_n e^{in\theta} + \overline{a_n} e^{-in\theta})$ continuously differentiable.

The main result of [1] is a special case of the following theorem: the case where $\widehat{a}(\theta) = -\cos(\theta)$ and $\psi_0 = e_0$.

Theorem 1. *Suppose that the matrix (3) represents an operator A on $\ell^2(\mathbb{Z})$ of the form $\mathcal{F}\mathcal{M}[\widehat{a}]\mathcal{F}^*$, where $\mathcal{M}[\widehat{a}]$ denotes the operator on $L^2(\mathbb{T}, \frac{d\theta}{2\pi})$ of multiplication by a measurable real-valued function*

$\widehat{a}(\theta)$. Suppose that $\widehat{a}'(\theta) = \frac{d}{d\theta}\widehat{a}(\theta)$ is defined almost everywhere with respect to Lebesgue measure $d\theta$. Let ψ_0 be any unit vector in $\ell^2(\mathbb{Z})$ and define

$$P_t(n) \;=\; \left|\langle e_n, e^{-itA}\psi_0\rangle\right|^2 \;, \tag{4}$$

where e_n is the n^{th} standard basis vector in $\ell^2(\mathbb{Z})$. Let $\mathbb{P}_t[\psi_0]$ be the probability measure

$$\mathbb{P}_t[\psi_0](dx) \;=\; \sum_{n\in\mathbb{Z}} P_t(n)\delta(x-n/t) \tag{5}$$

on $\mathbb{R}$, where $\delta(x-n/t)$ denotes the Dirac delta distribution at n/t.

Then the probability measures $\mathbb{P}_t[\psi_0]$ converge weakly as $t \longrightarrow \infty$ to the probability measure $\mathbb{P}[\psi_0]$ defined on measurable subsets $X \subset \mathbb{R}$ by

$$\mathbb{P}[\psi_0](X) \;=\; \frac{1}{2\pi}\int_{\left\{\theta:\; -\widehat{a}'(\theta)\in X\right\}} \left|(\mathcal{F}^*\psi_0)(\theta)\right|^2 d\theta \;. \tag{6}$$

Proof: We will show that the "characteristic functions" of the probability measures (5) converge to the characteristic function of the probability measure (6), for this implies the weak convergence of the probability measures themselves [9, Section XIII-1]. The characteristic functions $\Phi_t(\omega)$ of the probability measures $\mathbb{P}_t[\psi_0]$ in (4) are

$$\begin{aligned}\Phi_t(\omega) \;&\equiv\; \int e^{i\omega x}\mathbb{P}_t[\psi_0](dx) \;=\; \sum_{n\in\mathbb{Z}} P_t(n)e^{i\omega n/t} \;=\; \sum_{n\in\mathbb{Z}} e^{i\omega n/t}\left|\langle e_n, e^{-itA}\psi_0\rangle\right|^2 \\ &=\; \left\langle e^{-itA}\psi_0,\; E_{\omega/t}e^{-itA}\psi_0\right\rangle \;=\; \left\langle \psi_0,\; e^{itA}E_{\omega/t}e^{-itA}\psi_0\right\rangle \;,\end{aligned} \tag{7}$$

where E_x denotes the multiplication operator $(E_x\psi)(n) = e^{inx}\psi(n)$ on $\ell^2(\mathbb{Z})$. To show that these characteristic functions converge, we will take Fourier transforms.

Let $\mathcal{M}[-\widehat{a}']$ denote the multiplication operator $(\mathcal{M}[-\widehat{a}']f)(\theta) = -\widehat{a}'(\theta)f(\theta)$ and let

$$H = \mathcal{F}\mathcal{M}[-\widehat{a}']\mathcal{F}^* \;. \tag{8}$$

Note that H may be an *unbounded* self-adjoint operator on $\ell^2(\mathbb{Z})$. We claim that

$$\lim_{t\to\infty} e^{itA}E_{\omega/t}e^{-itA}\psi \;=\; e^{i\omega H}\psi \tag{9}$$

for all $\psi \in \ell^2(\mathbb{Z})$. To prove this claim, first verify that

$$(\mathcal{F}^*e^{itA}\mathcal{F}f)(\theta) \;=\; (e^{it\mathcal{F}^*A\mathcal{F}}f)(\theta) \;=\; e^{it\widehat{a}(\theta)}f(\theta) \tag{10}$$

$$(\mathcal{F}^*E_{\omega/t}\mathcal{F}f)(\theta) \;=\; f(\theta+\omega/t) \tag{11}$$

for all $f \in L^2(\mathbb{T}, \frac{d\theta}{2\pi})$. Supposing that $(\mathcal{F}^*\psi)(\theta)$ is a continuous function on $\mathbb{T}$, we calculate that

$$\begin{aligned}\lim_{t\to\infty}(\mathcal{F}^*e^{itA}E_{\omega/t}e^{-itA}\psi)(\theta) \;&=\; \lim_{t\to\infty}((\mathcal{F}^*e^{itA}\mathcal{F})(\mathcal{F}^*E_{\omega/t}\mathcal{F})(\mathcal{F}^*e^{-itA}\mathcal{F})\mathcal{F}^*\psi)(\theta) \\ &=\; \lim_{t\to\infty} e^{it\widehat{a}(\theta)}e^{-it\widehat{a}(\theta+\omega/t)}(\mathcal{F}^*\psi)(\theta+\omega/t) \\ &=\; e^{-i\omega\widehat{a}'(\theta)}(\mathcal{F}^*\psi)(\theta)\end{aligned} \tag{12}$$

at almost every θ by (10) and (11). Since $\mathcal{F}^*\psi$ is bounded, the functions that converge pointwise in (12) also converge in $L^2(\mathbb{T}, \frac{d\theta}{2\pi})$ by Lebesgue's Bounded Convergence Theorem. The continuity of $\mathcal{F}$ from $L^2(\mathbb{T}, \frac{d\theta}{2\pi})$ to $\ell^2(\mathbb{Z})$ implies that

$$\lim_{t\to\infty} e^{itA} E_{\omega/t} e^{-itA}\psi \;=\; \mathcal{F} e^{i\omega\mathcal{M}[-\widehat{a}']}\mathcal{F}^*\psi \;=\; e^{i\omega H}\psi$$

as claimed in (9). This verifies the claim when $\mathcal{F}^*\psi$ is a continuous function; the general claim follows by a straightforward density argument.

Applying the claim (9) in (7) yields

$$\lim_{t\to\infty} \Phi_t(\omega) \;=\; \left\langle \psi_0,\; e^{i\omega H}\psi_0 \right\rangle .$$

Using the unitary isomorphism $\mathcal{F}$ and the definition (8) of H one finds

$$\begin{aligned}
\Phi(\omega) \;&\equiv\; \lim_{t\to\infty} \Phi_t(\omega) \;=\; \left\langle \psi_0,\; e^{i\omega H}\psi_0 \right\rangle_{\ell^2} \;=\; \left\langle \mathcal{F}^*\psi_0,\; (\mathcal{F}^* e^{i\omega H}\mathcal{F})\mathcal{F}^*\psi_0 \right\rangle_{L^2} \\
&=\; \left\langle \mathcal{F}^*\psi_0,\; e^{i\omega\mathcal{F}^* H\mathcal{F}}\mathcal{F}^*\psi_0 \right\rangle_{L^2} \;=\; \left\langle \mathcal{F}^*\psi_0,\; e^{i\omega\mathcal{M}[-\widehat{a}']}\mathcal{F}^*\psi_0 \right\rangle_{L^2} \\
&=\; \int_{\mathbb{T}} e^{-i\omega\widehat{a}'(\theta)} \left|(\mathcal{F}^*\psi_0)(\theta)\right|^2 \tfrac{d\theta}{2\pi} \;.
\end{aligned}$$

This is the characteristic function of the probability measure $\mathbb{P}[\psi_0]$ defined in (6). □

References

[1] N. Konno. Continuous-time quantum walk on the line. To appear in Physical Review E. *Manuscript: quant-ph/0408140* (2004)

[2] N. Konno. Quantum random walks in one dimension. *Quantum Information Processing* 1: 345-354 (2002)

[3] N. Konno. A new type of limit theorems for the one-dimensional quantum random walk. To appear in Journal of the Mathematical Society of Japan. *Manuscript: quant-ph/0206103* (2002)

[4] G. Grimmett, S. Janson, P.F. Scudo. Weak limits for quantum random walks. *Physical Review E* 69: 026119 (2004)

[5] A.D. Gottlieb, S. Janson, P.F. Scudo. Convergence of quantum walks in $\mathbb{R}^d$. *Infinite Dimensional Analysis, Quantum Probability and Related Topics* 8 (1): 129-140 (2005)

[6] A.M. Childs, E. Farhi, S. Gutmann. An example of the difference between quantum and classical random walks. *Quantum Information Processing* 1: 35 - 43 (2002)

[7] C. Moore and A. Russell. Quantum walks on the hypercube. *Proceedings of the Sixth International Workshop on Randomization and Approximation Techniques in Computer Science* (RANDOM '02) *Manuscript: quant-ph/0104137* (2002)

[8] H. Gerhardt and J. Watrous. Continuous-time quantum walks on the symmetric group. *Proceeding of the Seventh International Workshop on Randomization and Approximation Techniques in Computer Science* (RANDOM '03) *Manuscript: quant-ph/0305182* (2003)

[9] W. Feller. *An Introduction to Probability Theory and its Applications II*. Second edition, John Wiley & Sons, New York (1971)