Convergence of coined quantum walks on $\mathbb{R}^d$

Alex D. Gottlieb[*], Svante Janson[†], and Petra F. Scudo[‡]

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Abstract

Coined quantum walks may be interpreted as the motion in position space of a quantum particle with a spin degree of freedom; the dynamics are determined by iterating a unitary transformation which is the product of a spin transformation and a translation conditional on the spin state. Coined quantum walks on $\mathbb{Z}^d$ can be treated as special cases of coined quantum walks on $\mathbb{R}^d$. We study quantum walks on $\mathbb{R}^d$ and prove that the sequence of rescaled probability distributions in position space associated to the unitary evolution of the particle converges to a limit distribution.

1 Introduction

Several kinds of quantum walks have recently been studied by many authors; a nice overview is given by [10]. So-called "coined quantum walks" on finite graphs, introduced in [1], are proving to be of some interest in quantum informatics, where they have been used to devise fast search algorithms [3, 10, 15]. Quantum walks of the type considered in this article, namely, coined quantum walks on $\mathbb{Z}^d$ or $\mathbb{R}^d$, were first introduced in [4], though [2] and [13] can be considered as precursors in some respects.

A coined quantum walk describes the evolution of a quantum system under iteration of a certain kind of unitary map. The state of the system is a vector in a product Hilbert space, having position degrees of freedom and an internal degree of freedom such as spin or polarization. A step of the walk consists of a unitary transformation of the spin degree of freedom, which one may think of as "tossing a quantum coin", followed by a translation conditional upon the state of the coin. Here we restrict our attention to walks on $\mathbb{Z}^d$ or $\mathbb{R}^d$ and we prove that the position distribution of the quantum walker, properly rescaled, converges as the number of steps tends to infinity. This type of convergence was first discovered by N. Konno [11, 12] in the case of one-dimensional lattices $\mathbb{Z}$. A different proof of Konno's theorem was given in [7], generalizing the convergence to quantum walks on higher dimensional lattices $\mathbb{Z}^d$. In this article we present a further generalization of the result to quantum walks on $\mathbb{R}^d$.

We start by reviewing some basic definitions and stating Konno's theorem for a coined quantum walk on $\mathbb{Z}$.

[*]Wolfgang Pauli Institute c/o Institut für Mathematik, Universität Wien, Nordbergstraße 15, 1090 Wien, Austria (alex@alexgottlieb.com).

[†]Department of Mathematics, Uppsala University, PO Box 480, S-751 06 Uppsala, Sweden (svante.janson@math.uu.se).

[‡]Department of Physics, Technion—Israel Institute of Technology, 32000 Haifa, Israel (scudo@tx.technion.ac.il).

A simple quantum walk on $\mathbb{Z}$ can be defined as a sequence

$$\psi,\ U\psi,\ U^2\psi,\ U^3\psi,\ \ldots, \tag{1}$$

of unit vectors in the Hilbert space $\ell^2(\mathbb{Z}) \otimes \mathbb{C}^2$ obtained by iterating a unitary operator U of the form

$$U = S(I \otimes C)\ . \tag{2}$$

In (2), I denotes the identity operator on $\ell^2(\mathbb{Z})$, C denotes a unitary operator on $\mathbb{C}^2$, and S denotes the "conditional shift" operator

$$\begin{aligned} S(s_m \otimes e_1) &= s_{m+1} \otimes e_1 \\ S(s_m \otimes e_2) &= s_{m-1} \otimes e_2\ , \end{aligned} \tag{3}$$

where e_1 and e_2 are the standard basis vectors for $\mathbb{C}^2$ and s_m is the vector in $\ell^2(\mathbb{Z})$ whose m^{th} member is 1 and all other members are 0. Since the vectors of the sequence (1) are normalized, the numbers

$$P_n(m)\ =\ \big|\langle s_m \otimes e_1,\ U^n\psi\rangle\big|^2 + \big|\langle s_m \otimes e_2,\ U^n\psi\rangle\big|^2 \tag{4}$$

satisfy $\sum_m P_n(m) = 1$ and thus define a sequence of probability measures on $\mathbb{Z}$. Note that the only variable considered here is the position of the walker; the internal degree of freedom is disregarded by summing over both states in the coin space. Konno's theorem [12] states that the probability measures

$$\sum_{m\in\mathbb{Z}} P_n(m)\ \delta_{m/n} \tag{5}$$

converge weakly as $n \longrightarrow \infty$ to a probability measure that depends on the initial state ψ (here $\delta_{m/n}$ denotes a point-mass at m/n).

The dynamics described in (1), (2), (3) is reminiscent of simple random walk on $\mathbb{Z}$, though there are a few important differences. As in ordinary random walks, the rule (3) for stepping left or right is the same at all locations $m \in \mathbb{Z}$, that is, the process is spatially homogeneous. Unlike ordinary random walks, the probability distributions (4) for the system's position are not related by Markov transitions. Similarly to random walk, the sequence of rescaled position distributions (5) converges weakly, but unlike random walks, the weak limit is obtained by rescaling by a factor of $1/n$ rather than $1/\sqrt{n}$ and the limit distribution depends on the initial state (and is not a normal distribution).

In the next sections we state and prove a generalization of Konno's theorem in which (i) the walk takes place in d-dimensional space $\mathbb{R}^d$, (ii) any finite number s of conditional translations are allowed at each step, and (iii) the translations are not assumed to generate a lattice in $\mathbb{R}^d$. This theorem strictly subsumes the results proved in [12, 7] for quantum walks on the d-dimensional lattice $\mathbb{Z}^d$, because the latter may be regarded as special cases of quantum walks on $\mathbb{R}^d$ as indicated after the statement of Theorem 1.

2 General quantum walks convergence theorem

Broadly speaking, a quantum walk is characterized by the unitary operator U that generates the walk, U being a particular kind of unitary operator on a Hilbert space $L^2(\mathbb{Z}^d)\otimes\mathbb{C}^s$ or $L^2(\mathbb{R}^d)\otimes\mathbb{C}^s$, the former for quantum walks on $\mathbb{Z}^d$ and the latter for quantum walks on $\mathbb{R}^d$. We now focus our discussion onto quantum walks on $\mathbb{R}^d$, for quantum walks on $\mathbb{Z}^d$ are easily embedded into the framework of walks on $\mathbb{R}^d$.

Let $\mathcal{H} = L^2(\mathbb{R}^d) \otimes \mathbb{C}^s$. There is a natural isomorphism between $L^2(\mathbb{R}^d) \otimes \mathbb{C}^s$ and $L^2(\mathbb{R}^d, \mathbb{C}^s)$; it will be helpful to represent members of $\mathcal{H}$ as members of $L^2(\mathbb{R}^d, \mathbb{C}^s)$, and indeed to represent members of $\mathbb{C}^s$ as column vectors for the purpose of interpreting matrix operations. Let C denote a unitary "coin tossing operator" on the "coin space" $\mathbb{C}^s$ and let I_s denote the identity operator on $\mathbb{C}^s$. Let $e_1, e_2, \ldots, e_s$ be the standard ordered basis of $\mathbb{C}^s$. The steps of the quantum walk involve a "conditional translation" operator T on $\mathcal{H}$ defined by

$$T(\psi \otimes e_j) \;=\; T_{v_j}\psi \otimes e_j \;, \tag{6}$$

where T_{v_j} denotes translation by v_j in $\mathbb{Z}^d$ or $\mathbb{R}^d$, i.e., $(T_{v_j}\psi)(x) = \psi(x - v_j)$. The vectors v_j are arbitrary fixed vectors in $\mathbb{Z}^d$ or $\mathbb{R}^d$. A step of the quantum walk is effected by a unitary operator

$$U \;=\; T(I \otimes C) \;, \tag{7}$$

where I denotes the identity operator on $L^2(\mathbb{Z}^d)$ or $L^2(\mathbb{R}^d)$.

The operator U generates the quantum walk. In the Schrödinger picture, the quantum walk may be thought of as a sequence

$$\rho,\; U\rho U^*,\; U^2\rho U^{*2},\; U^3\rho U^{*3},\; \ldots \tag{8}$$

of density operators on $\mathcal{H}$. (Recall that a density operator is a nonnegative trace class operator with normalization $\mathrm{Tr}(\rho) = 1$ [6]. The density operator ρ for the normalized pure state $\psi \in \mathcal{H}$ has integral kernel $\psi(x)\overline{\psi(y)}$. Thus, the definition (8) of quantum walk in terms of density operators generalizes the original definition (1) for pure states ψ.) The probability measures (4) can be expressed in terms of density operators instead of wavefunctions as follows. Given an initial density operator ρ on $\mathcal{H}$ and any $n \in \mathbb{N}$, there is a probability measure $\mathbb{P}_{\rho,n}$ on $\mathbb{Z}^d$ or $\mathbb{R}^d$ that may be defined as a linear functional on $C_0(\mathbb{Z}^d)$ or $C_0(\mathbb{R}^d)$ by the formula

$$\mathbb{P}_{\rho,n} f \;=\; \mathrm{Tr}(U^n \rho U^{*n}(m[f(\,*\,)] \otimes I_s)) \;, \tag{9}$$

where C_0 denotes the set of continuous functions that tend to 0 at ∞, f is an element of this set, and $m[f(\,*\,)]$ is the multiplication operator $\psi(x) \longmapsto f(x)\psi(x)$ on $L^2(\mathbb{R}^d)$. Formula (9) may be written as

$$\mathbb{P}_{\rho,n} f \;=\; \mathrm{Tr}(\mathrm{Tr}_{\mathbb{C}^s}(U^n \rho U^{*n}) m[f(\,*\,)]) \;, \tag{10}$$

where $\mathrm{Tr}_{\mathbb{C}^s}$ denotes the partial trace; for the special case discussed in the Introduction, one may verify that $\mathbb{P}_{\rho,n}$ is the same as P_n of (4) when ρ is a pure state ψ. The quantum walk as such is the sequence of density operators (8) and the corresponding probabilities (10), which express probabilites concerning the position of a "particle" without regard to its internal "spin" state in $\mathbb{C}^s$.

One observes that the probability measures $\mathbb{P}_{\rho,n}$ spread out in $\mathbb{Z}^d$ or $\mathbb{R}^d$ as n increases. However, we will discover that dilating each of the $\mathbb{P}_{\rho,n}$ by a factor of $1/n$ produces in a sequence of probability measures that converges weakly. In other words, if X_n is a random vector describing the position of the quantum walk after n steps, then the sequence X_n/n converges in distribution.

Now we are prepared to state a generalized version of Konno's theorem [11, 12, 7]. In the following, $C_b(\mathbb{R}^d)$ denotes the space of bounded continuous functions on $\mathbb{R}^d$, and a sequence of probability measures is said to converge weakly if the measures converge pointwise as functionals on $C_b(\mathbb{R}^d)$ [5].

Theorem 1. *Let U be a unitary operator on $\mathcal{H} = L^2(\mathbb{R}^d) \otimes \mathbb{C}^s$ of the form* (7).

There exists a spectral measure $P(dx)$ on $\mathbb{R}^d$ such that for any density operator ρ on $\mathcal{H}$, the probability measures $\mathbb{P}^{(n)}_{\rho,n}$ defined by

$$\mathbb{P}^{(n)}_{\rho,n} f \;=\; \mathrm{Tr}\big(\mathrm{Tr}_{\mathbb{C}^s}(U^n \rho U^{*n}) m[f(\,*\,/n)]\big) \tag{11}$$

converge weakly as $n \longrightarrow \infty$ to the probability measure $\mathbb{P}_\rho(E) = \mathrm{Tr}(\rho P(E))$.

We will prove this theorem — and somewhat more — in the next section, but first it is appropriate to explain how Theorem 1 subsumes Konno's theorem for walks on the lattice. Convergence of quantum walks on $\mathbb{R}^d$ implies convergence of quantum walks on $\mathbb{Z}^d$ because quantum walks on $\mathbb{Z}^d$ can be identified with quantum walks on $\mathbb{R}^d$ that have integral steps. Indeed, the space $L^2(\mathbb{Z}^d)$ can be identified with the subspace $\mathbb{L} \subset L^2(\mathbb{R}^d)$ consisting of functions that are constant on each unit cube centered at a lattice point. The subspace $\mathbb{L}$ is invariant under translation by any lattice vector in $\mathbb{Z}^d$, so that a quantum walk on $\mathbb{Z}^d$ may be viewed as a quantum walk on $\mathbb{R}^d$ whose initial density operator is supported on the subspace $\mathbb{L} \otimes \mathbb{C}^s$ of $L^2(\mathbb{R}^d) \otimes \mathbb{C}^s$. Convergence of the $\mathbb{P}^{(n)}_{\rho,n}$ for the walk on $\mathbb{R}^d$ then implies the convergence considered in [12, 7] for walks on $\mathbb{Z}^d$.

3 Proof of Theorem 1

Theorem 1 is formulated in the Schrödinger picture, where the evolution is applied to the state of the system. In the Heisenberg picture, where the the state of the system remains constant and the physical observables evolve, the quantum walk concerns the map

$$X \;\longmapsto\; X,\; U^*XU,\; U^{*2}XU^2,\; U^{*3}XU^3,\; \ldots$$

from bounded operators X on $\mathcal{H}$ to sequences of bounded operators. We are interested in operators X that represent physical observables of position alone, namely, the operators of the form $m[f(\,*\,)] \otimes I_s$. Theorem 1 is the consequence of a stronger, dual formulation in the Heisenberg picture. In the following, the notation $\mathrm{s}\cdot\lim$ designates the limit in the strong operator topology, the topology in which nets of operators converge if and only if they converge pointwise as functions on $\mathcal{H}$.

Theorem 2. *Let U be a unitary operator on $\mathcal{H} = L^2(\mathbb{R}^d) \otimes \mathbb{C}^s$ of the form (7).*

There exists a spectral measure $P(dx)$ on $\mathbb{R}^d$ and a corresponding family of commuting bounded self-adjoint operators $V_1, \ldots, V_d$ such that

$$\mathrm{s}\cdot\lim_{n\to\infty} U^{*n}(m[f(\,*\,/n)] \otimes I_s)U^n \;=\; \int_{\mathbb{R}^d} f(x)P(dx) \;=\; f(V_1, \ldots, V_d) \tag{12}$$

for all $f \in C_b(\mathbb{R}^d)$.

Theorem 1 follows from Theorem 2 and the observation that the strong operator topology is stronger than the weak* topology on bounded subsets of $\mathcal{B}(\mathcal{H})$. That is, on bounded subsets of $\mathcal{B}(\mathcal{H})$, all linear functionals on $\mathcal{B}(\mathcal{H})$ of the form $X \longmapsto \mathrm{Tr}(TX)$ for some trace class operator T are strongly continuous. Since the operators $U^{*n}(m[f(\,*\,/n)] \otimes I_s)U^n$ are bounded in norm and converge strongly to $\int f(x)P(dx)$, it follows that

$$\begin{aligned}
\lim_{n\to\infty} \mathbb{P}^{(n)}_{\rho,n} f(x) \;&=\; \lim_{n\to\infty} \mathrm{Tr}\big(\rho\, U^{*n}(m[f(\,*\,/n)] \otimes I_s)U^n\big) \\
&=\; \mathrm{Tr}\left(\rho\, \big(\mathrm{s}\cdot\lim_{n\to\infty} U^{*n}(m[f(\,*\,/n)] \otimes I_s)U^n\big)\right) \\
&=\; \mathrm{Tr}\left(\rho \int f(x)P(dx)\right) \;=\; \int f(x)\,\mathrm{Tr}(\rho P(dx))\;.
\end{aligned} \tag{13}$$

Thus, it suffices to prove Theorem 2. Here is the plan of the proof: Note that, for each n, the map

$$\mathbf{U}_n : \omega \longmapsto U^{*n}(m[e^{i\omega\cdot(\;*\;)/n}] \otimes I_s)U^n \tag{14}$$

is a strongly continuous unitary representation of $\mathbb{R}^d$ on $L^2(\mathbb{R}^d, \mathbb{C}^s)$, i.e., $\mathbf{U}_n$ is a group homomorphism from $\mathbb{R}^d$ to the unitary operators on $\mathcal{H}$ such that $\mathbf{U}_n(\omega)\psi$ is continuous in ω for each $\psi \in \mathcal{H}$. We will prove that the $\mathbf{U}_n(\omega)$ converge pointwise in the strong operator topology as $n \longrightarrow \infty$ and we will identify the limit as a uniformly continuous unitary representation of $\mathbb{R}^d$. By Stone's spectral theorem there exists a spectral measure $P(dx)$ on $\mathbb{R}^d$ such that

$$\mathrm{s}\cdot\lim_{n\to\infty} U^{*n}(m[e^{i\omega\cdot(*)/n}] \otimes I_s)U^n \;=\; \int_{\mathbb{R}^d} e^{i\omega\cdot x} P(dx)$$

for all $\omega \in \mathbb{R}^d$. This proves that

$$\mathrm{s}\cdot\lim_{n\to\infty} U^{*n}(m[f(\;*\;/n)] \otimes I_s)U^n \;=\; \int f(x)P(dx) \tag{15}$$

for all $f \in \mathrm{span}\{e^{i\omega\cdot x} : \omega \in \mathbb{R}^d\}$. Finally, to complete the proof of Theorem 2, we will extend the convergence in (15) to all functions $f \in C_b(\mathbb{R}^d)$.

We begin by showing that $\mathbf{U}_n(\omega)$ converges strongly at each $\omega \in \mathbb{R}^d$. To do this, we will first prove that the infinitesimal generators of these unitary groups converge on a dense subset of $\mathcal{H}$ to a bounded skew-Hermitian operator, and then invoke the Trotter–Kato Theorem.

For arbitrary but fixed $\omega \in \mathbb{R}^d$, the one-parameter unitary group $\{\mathbf{U}_n(t\omega)\}_{t\in\mathbb{R}}$ has infinitesimal generator

$$\mathcal{G}_n \;=\; \tfrac{1}{n}U^{*n}(m[i\omega\cdot(*)] \otimes I_s)U^n. \tag{16}$$

Observe that if $D(\omega)$ is the operator on $\mathbb{C}^s$ represented by the diagonal matrix

$$D(\omega) \;=\; \begin{bmatrix} \omega\cdot v_1 & 0 & \cdots & 0 \\ 0 & \omega\cdot v_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \omega\cdot v_s \end{bmatrix},$$

then, for any $f \in L^2(\mathbb{R}^d)$,

$$T^*(m[\omega\cdot(*)] \otimes I_s)T(f \otimes e_j) = m[\omega\cdot(* + v_j)] \otimes I_s(f \otimes e_j) = \Big(m[\omega\cdot(*)] \otimes I_s + I \otimes D(\omega)\Big)(f \otimes e_j)$$

and hence

$$\begin{aligned} U^*(m[i\omega\cdot(*)] \otimes I_s)U \;&=\; (I \otimes C^*)T^*(m[i\omega\cdot(*)] \otimes I_s)T(I \otimes C) \\ &=\; m[i\omega\cdot(*)] \otimes I_s \;+\; i(I \otimes C^*D(\omega)C)\;. \end{aligned} \tag{17}$$

Applying (17) recursively in (16) shows that

$$\mathcal{G}_n \;=\; \tfrac{1}{n}m[i\omega\cdot(*)] \otimes I_s \;+\; i\,\frac{1}{n}\sum_{j=0}^{n-1} U^{*j}(I \otimes C^*D(\omega)C)U^j\;. \tag{18}$$

The first term on the right-hand side of (18) is an unbounded multiplication operator; as $n \longrightarrow \infty$ these operators converge to the zero operator on the dense subset of $L^2(\mathbb{R}^d, \mathbb{C}^s)$ consisting of functions of bounded support. The second term on the right-hand side of (18) is a bounded operator; we will prove that these bounded operators converge strongly as $n \longrightarrow \infty$.

We take Fourier transforms to identify the limit of the operators

$$\frac{1}{n}\sum_{j=0}^{n-1} U^{*j}(I \otimes C^* D(\omega) C) U^j \ . \tag{19}$$

Let $\mathcal{F}$ denote the Fourier transform

$$\mathcal{F}(\psi)(k) \ = \ (2\pi)^{-d/2} \int_{\mathbb{R}^d} \psi(x) e^{-ik\cdot x} dx \tag{20}$$

on $\mathbb{R}^d$. The map $\mathcal{F}$ has a unique extension from $L^1(\mathbb{R}^d) \cap L^2(\mathbb{R}^d)$ to a unitary transformation from $L^2(\mathbb{R}^d)$ onto an isomorphic space $\widehat{L^2}(\mathbb{R}^d)$. This unitary isomorphism will also be denoted by $\mathcal{F}$, and its inverse by $\mathcal{F}^*$. The spaces $L^2(\mathbb{R}^d) \otimes \mathbb{C}^s$ and $\widehat{L^2}(\mathbb{R}^d) \otimes \mathbb{C}^s$ are mapped onto one another via the unitary transformations $\mathcal{F} \otimes I_s$ and $\mathcal{F}^* \otimes I_s$. We will denote $\mathcal{F} \otimes I_s$ by $\widetilde{\mathcal{F}}$ from now on. The operator U of (7) is unitarily equivalent to the operator $\widehat{U} = \widetilde{\mathcal{F}} U \widetilde{\mathcal{F}}^*$ on $\widehat{\mathcal{H}}$. We will think of $\widehat{\mathcal{H}}$ (the momentum space of the system) as $L^2(\mathbb{R}^d, \mathbb{C}^s)$, that is, we represent vectors in $\widehat{\mathcal{H}}$ by square-integrable column-vector valued functions on $\mathbb{R}^d$. Then the operator $\widehat{U}$ may then be represented by a "matrix-multiplication operator"

$$(\widehat{U}\phi)(k) \ = \ \widehat{U}_k \phi(k)$$

with

$$\widehat{U}_k \ = \ \begin{bmatrix} e^{-ik\cdot v_1} & 0 & \cdots & 0 \\ 0 & e^{-ik\cdot v_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & e^{-ik\cdot v_s} \end{bmatrix} \begin{bmatrix} C_{11} & C_{12} & \cdots & C_{1s} \\ C_{21} & C_{22} & \cdots & C_{2s} \\ \vdots & \vdots & \ddots & \vdots \\ C_{s1} & C_{s2} & \cdots & C_{ss} \end{bmatrix} \tag{21}$$

where the C_{jk} denote the matrix elements of the coin toss operator C. The Fourier transform of the operator $\frac{1}{n}\sum_{j=0}^{n-1} U^{*j}(I \otimes (C^* D(\omega) C)) U^j$ is the matrix-multiplication operator

$$\phi(k) \ \longmapsto \ \frac{1}{n}\sum_{j=0}^{n-1} \widehat{U}_k^{*j} C^* D(\omega) C \widehat{U}_k^j \ \phi(k) \ . \tag{22}$$

For fixed $k \in \mathbb{R}^d$ the map $X \longmapsto \widehat{U}_k^* X \widehat{U}_k$ is a unitary operator on the space of $s \times s$ matrices endowed with the inner product $\langle Y, X \rangle = \mathrm{Tr}(Y^* X)$. The Mean Ergodic Theorem implies that the matrices in (22) converge as $n \longrightarrow \infty$ to the orthogonal projection of $C^* D(\omega) C$ onto the subspace of $s \times s$ matrices that commute with $\widehat{U}_k$. That is,

$$W_k(\omega) \ = \ \lim_{n\to\infty} \frac{1}{n}\sum_{j=0}^{n-1} \widehat{U}_k^{*j} (C^* D(\omega) C) \widehat{U}_k^j \tag{23}$$

is the unique matrix that commutes with $\widehat{U}_k$ and satisfies

$$\mathrm{Tr}(N^* W_k(\omega)) \ = \ \mathrm{Tr}(N^* C^* D(\omega) C) \tag{24}$$

for all matrices N that commute with $\widehat{U}_k$. Since $C^* D(\omega) C$ is Hermitian and since N commutes with $\widehat{U}_k$ if and only if N^* commutes with $\widehat{U}_k$, taking adjoints in (24) shows that the matrices $W_k(\omega)$ are

Hermitian. From (21) and (23) it is seen that $W_k(\omega)$ is a limit of continuous functions of k, hence it is a measurable function of k. Moreover, the operator norm of each matrix on the right-hand side of (23) does not exceed the operator norm of $D(\omega)$, which is independent of k, and the limit $W_k(\omega)$ enjoys the same uniform bound. Thanks to these bounds, Lebesgue's Dominated Convergence Theorem implies that the operators (22) converge strongly to the matrix-multiplication operator $\mathcal{W}(\omega)$ defined by

$$(\mathcal{W}(\omega)\phi)(k) \;=\; W_k(\omega)\phi(k) \tag{25}$$

on $\widehat{\mathcal{H}}$, a bounded Hermitian operator. Transforming back to operators on $\mathcal{H}$, we conclude that the operators (19) converge strongly to

$$\mathcal{V}(\omega) = \widetilde{\mathcal{F}}^{*}\mathcal{W}(\omega)\widetilde{\mathcal{F}}. \tag{26}$$

We have now shown that the generators (18) converge to $i\mathcal{V}(\omega)$ on a dense subset of $\mathcal{H}$. By the Trotter–Kato Theorem [14, Theorem 4.5], the operators $\mathbf{U}_n(t\omega)$ converge strongly to $e^{it\mathcal{V}(\omega)}$ for each $t \in \mathbb{R}$. In particular, $\mathbf{U}_n(\omega)$ converges strongly to $e^{i\mathcal{V}(\omega)}$, i.e.,

$$\mathrm{s}\cdot\lim_{n\to\infty} U^{*n}(m[e^{i\omega\cdot(*)/n}]\otimes I_s)U^n \;=\; e^{i\mathcal{V}(\omega)} \;.$$

It follows from (23), (25) and (26) that $\mathcal{V}(\omega)$ depends linearly on $\omega \in \mathbb{R}^d$; in particular, $\omega \longmapsto \mathcal{V}(\omega)$ is continuous. Moreover, $\omega \longmapsto e^{i\mathcal{V}(\omega)}$ is a d-parameter group of unitary operators on $\mathcal{H}$ because each $\omega \longmapsto \mathbf{U}_n(\omega)$ is. It follows that $e^{i\mathcal{V}(\omega)}$ is a uniformly continuous d-parameter unitary group. Stone's spectral theorem for one-parameter unitary groups can be generalized to d-parameter unitary groups: for any strongly continuous d-parameter unitary group $\mathbf{U}(\omega)$ there exists a spectral measure $P(dx)$ on $\mathbb{R}^d$ such that

$$\mathbf{U}(\omega) \;=\; \int_{\mathbb{R}^d} e^{i\omega\cdot x}P(dx) \;,$$

and $P(dx)$ has bounded support if $\mathbf{U}$ is uniformly continuous (see, e.g., [8, Chapter 2.4]). For one-parameter groups $e^{i\omega V}$, $P(dx)$ is just the spectral measure associated to the self-adjoint operator V, and in general P is the spectral measure of a d-tuple $(V_1,\ldots,V_d)$ of commuting bounded operators. Let $P(dx)$ denote the spectral measure associated to $e^{i\mathcal{V}(\omega)}$. What we have shown up to this point is that

$$\mathrm{s}\cdot\lim_{n\to\infty} U^{*n}(m[e^{i\omega\cdot(*)/n}]\otimes I_s)U^n \;=\; e^{i\mathcal{V}(\omega)} \;=\; \int_{\mathbb{R}^d} e^{i\omega\cdot x}P(dx) \tag{27}$$

for all $\omega \in \mathbb{R}^d$.

To complete the proof of Theorem 2, we have to extend to all functions in $C_b(\mathbb{R}^d)$ the convergence (27) just established for functions $e^{i\omega\cdot x}$. By linearity, the assertion of the theorem holds for all $f \in \mathrm{span}\{e^{i\omega\cdot x} : \omega \in \mathbb{R}^d\}$. Let f be an arbitrary but fixed function in $C_b(\mathbb{R}^d)$ and define

$$\mathrm{L}[f,n](\psi) \;=\; U^{*n}(m[f(\,*\,/n)]\otimes I_s)U^n\psi$$

on $\mathcal{H}$. We want to prove that

$$\lim_{n\to\infty} \mathrm{L}[f,n](\psi) \;=\; \int f(x)P(dx)\psi$$

for all $\psi \in \mathcal{H}$. The sequence $\{\mathrm{L}[f,n]\}$ is equicontinuous on $\mathcal{H}$ thanks to the uniform bound

$$\|U^{*n}(m[f(\,*\,/n)]\otimes I_s)U^n\| \;=\; \|f\|_\infty \;,$$

so it suffices to prove the convergence of the sequence $\{\mathrm{L}[f,n]\}$ on a dense subset of $\mathcal{H}$. We will show that $\mathrm{L}[f,n](\psi)$ converges for all ψ that have bounded support.

We continue to represent members of $\mathcal{H}$ by functions in $L^2(\mathbb{R}^d,\mathbb{C}^s)$. Let $\psi\in\mathcal{H}$ have bounded support, in the sense that there exists $r>0$ such that $\psi(x)$ equals $\mathbf{0}\in\mathbb{C}^s$ when $|x|>r$. We claim that $\mathrm{L}[f,n]\psi$ tends to a limit. We may assume that ψ has norm 1 without loss of generality. Let

$$v \;=\; \max_{1\le j\le s}\left\{|v_j|\right\},$$

where the v_j are the translation vectors appearing in the definition (6) of T. Then $U^n\psi$ is supported on the ball of radius $r+nv$ in $\mathbb{R}^d$. For any $g\in C_b(\mathbb{R}^d)$,

$$\begin{aligned}\left\|\,\mathrm{L}[f,n]\psi-\mathrm{L}[g,n]\psi\right\| &= \left\|U^{*n}((m[f(\,*\,/n)]-m[g(\,*\,/n)])\otimes I_s)U^n\psi\right\|\\ &\le \sup_{|x|<r+v}\{|f(x)-g(x)|\}\end{aligned}\tag{28}$$

for all n because of the way that f and g are scaled. By the Stone–Weierstrass Theorem, the linear span of $\{e^{i\omega\cdot x}:\omega\in\mathbb{R}^d\}$ is dense in the space of continuous functions on any compact subset of $\mathbb{R}^d$, so $f(x)$ can be uniformly approximated within arbitrary $\epsilon>0$ on the ball of radius $r+v$ by some function $g_\epsilon\in\mathrm{span}\{e^{i\omega\cdot x}:\omega\in\mathbb{R}^d\}$. We know that each sequence $\mathrm{L}[g_\epsilon,n]\psi$ converges as $n\longrightarrow\infty$. On the other hand, $\mathrm{L}[g_\epsilon,n]\psi$ is within ϵ of $\mathrm{L}[f,n]\psi$ uniformly in n by (28). It follows that $\{\mathrm{L}[f,n]\psi\}$ converges as $n\longrightarrow\infty$. The limit is a continuous function of f and hence must agree everywhere with $\int f(x)P(dx)\psi=f(V_1,\ldots,V_d)$. This proves (12) for arbitrary $f\in C_b(\mathbb{R}^d)$ and concludes the proof of Theorem 2.

4 The limit distribution

In special cases there is a nice characterization of the limit distribution $\mathbb{P}_\rho$ of Theorem 1 in terms of the distribution of a certain random element of $\Omega=\mathbb{R}^d\times\{1,2,\ldots,s\}$.

Let $\widehat{\rho}\,=\widetilde{\mathcal{F}}\rho\widetilde{\mathcal{F}}^*$ be the density operator on $\widehat{\mathcal{H}}$ corresponding to ρ. This can be regarded as an integral operator $\widehat{\rho}\,f=\int_{\mathbb{R}^d}\widehat{\rho}\,(k,k')f(k')\,dk'$ with an $s\times s$ matrix valued kernel $\widehat{\rho}\,(k,k')$. Since $\widehat{\rho}$ is trace class, the diagonal $\widehat{\rho}\,(k,k)$ is well-defined a.e. and integrable. By Theorem 1 and (13), (27), we have (26),

$$\mathbb{P}_\rho[e^{i\omega\cdot x}]=\mathrm{Tr}\Big(\rho\int_{\mathbb{R}^d}e^{i\omega\cdot x}\,dP(x)\Big)=\mathrm{Tr}\Big(\rho e^{i\mathcal{V}(\omega)}\Big)=\mathrm{Tr}\Big(\widehat{\rho}\;e^{i\mathcal{W}(\omega)}\Big)=\int_{\mathbb{R}^d}\mathrm{Tr}\left[e^{iW_k(\omega)}\widehat{\rho}\,(k,k)\right]dk.$$

This shows that the characteristic function of the limit $\mathbb{P}_\rho$ in Theorem 1 is

$$\mathbb{P}_\rho[e^{i\omega\cdot x}]\;=\;\int_{\mathbb{R}^d}\mathrm{Tr}\left[e^{iW_k(\omega)}\widehat{\rho}\,(k,k)\right]dk,\tag{29}$$

with W_k given by (23) and (24).

We can better identify the limit measure $\mathbb{P}_\rho$ in cases where the matrices $\widehat{U}_k$ have s distinct eigenvalues $\lambda_1(k),\ldots,\lambda_s(k)$ for a.e. $k\in\mathbb{R}^d$. At a point k where there are s distinct eigenvalues, let $\psi_j(k)$ be a normalized eigenvector of $\widehat{U}_k$ with eigenvalue $\lambda_j(k)$, and let $P_k^{(j)}$ be the corresponding orthogonal projection onto the eigenspace. We may assume that the eigenvalues are numbered such that λ_j are continuous and differentiable in a neighborhood of k for each j [9][II-5.4], and we then define

$$\pi(k,j)\;=\;i\overline{\lambda_j(k)}\,\nabla\lambda_j(k),\tag{30}$$

where ∇ is the gradient with respect to $k\in\mathbb{R}^d$. Since $|\lambda_j(k)|\equiv 1$, the functions $i\overline{\lambda_j(k)}\nabla\lambda_j(k)$ are real-valued, and π is an a.e. defined map from $\mathbb{R}^d\times\{1,2,\ldots,s\}$ to $\mathbb{R}^d$.

Theorem 3. *Suppose that $\widehat{U}_k$ has s distinct eigenvalues at almost every k. Then,*

$$W_k(\omega) \;=\; \sum_{j=1}^{s} \big(\omega \cdot \pi(k,j)\big) P_k^{(j)} \tag{31}$$

and thus

$$\mathbb{P}_\rho[e^{i\omega\cdot x}] \;=\; \int_{\mathbb{R}^d} \sum_{j=1}^{s} e^{i\omega\cdot\pi(k,j)}\, \mathrm{Tr}[\widehat{\rho}\ (k,k) P_k^{(j)}] dk\ . \tag{32}$$

Proof. We may assume that the eigenvectors ψ_j are differentiable in a neighborhood of k [9][II-5.4]. Taking the directional derivative $\partial_\omega = \omega \cdot \nabla$ of $\widehat{U}_k \psi_j(k) = \lambda_j(k)\psi_j(k)$ we obtain, since (21) yields $\partial_\omega \widehat{U}_k = -iD(\omega)\widehat{U}_k$,

$$-iD(\omega)\widehat{U}_k\psi_j(k) + \widehat{U}_k \partial_\omega \psi_j(k) = \big(\partial_\omega \lambda_j(k)\big)\psi_j(k) + \lambda_j(k)\partial_\omega\psi_j(k). \tag{33}$$

Further,

$$\psi_j(k)^*\widehat{U}_k = \big(\widehat{U}_k^*\psi_j(k)\big)^* = \big(\overline{\lambda_j(k)}\psi_j(k)\big)^* = \lambda_j(k)\psi_j(k)^*$$

and thus (33) implies

$$\psi_j(k)^*\big(-iD(\omega)\widehat{U}_k\big)\psi_j(k) = \psi_j(k)^*\big(\partial_\omega\lambda_j(k)\big)\psi_j(k) = \partial_\omega\lambda_j(k). \tag{34}$$

Since $W_k(\omega)$ commutes with $\widehat{U}_k$ it is of the form $\sum_j a_j P_k^{(j)}$. Taking $N = N^* = \psi_j(k)\psi_j(k)^*$ in (24) yields, using $C^*D(\omega)C = \widehat{U}_k^* D(\omega)\widehat{U}_k$, (34) and (30),

$$\begin{aligned} a_j &= \mathrm{Tr}\Big(\psi_j(k)\psi_j(k)^* W_k(\omega)\Big) = \mathrm{Tr}\Big(\psi_j(k)\psi_j(k)^* C^* D(\omega) C\Big) = \psi_j(k)^*\widehat{U}_k^* D(\omega)\widehat{U}_k\psi_j(k) \\ &= \overline{\lambda_j(k)}\psi_j(k)^* D(\omega)\widehat{U}_k\psi_j(k) = i\overline{\lambda_j(k)}\,\partial_\omega\lambda_j(k) = \omega\cdot\pi(k,j). \end{aligned}$$

This gives (31), and (32) then follows from (29). □

Let $\widetilde{\mathbb{P}}_\rho$ denote the probability measure

$$\widetilde{\mathbb{P}}_\rho(dk,j) \;=\; \mathrm{Tr}[\widehat{\rho}\ (k,k)P_k^{(j)}]\ dk \tag{35}$$

on $\Omega = \mathbb{R}^d \times \{1,2,\ldots,s\}$. Then the right-hand side of (32) is the characteristic function of the induced probability measure $\widetilde{\mathbb{P}}_\rho \circ \pi^{-1}$ on $\mathbb{R}^d$, which identifies this probability measure as $\mathbb{P}_\rho$. In other words, if Y is a random element of Ω with the distribution $\widetilde{\mathbb{P}}_\rho$, then $\mathbb{P}_\rho$ is the distribution of the random variable $\pi(Y)$. We conclude with an interesting special case:

Corollary 1. *Suppose that the initial state is is of the form $\rho = \rho_0 \otimes \frac{1}{s}I_s$, a tensor product of a position density operator ρ_0 on $L^2(\mathbb{R}^d)$ with a maximally mixed coin state. Suppose further that the matrices $\widehat{U}_k$ have s distinct eigenvalues $\lambda_1(k),\ldots,\lambda_s(k)$ almost everywhere on $\mathbb{R}^d$. Then the limit $\mathbb{P}_\rho$ is the distribution of the random variable $\pi(Y_0,Z)$, where π is given by (30), Y_0 is a random vector in $\mathbb{R}^d$ with density function $\mathrm{Tr}\,\widehat{\rho_0}(k,k)$ and Z is uniformly distributed on $\{1,\ldots,s\}$, with Y_0 and Z independent.*

Proof. We have $\widehat{\rho}\ = \widehat{\rho_0} \otimes \frac{1}{s}I_s$ and, for the kernel, $\widehat{\rho}\ (k,k) = \widehat{\rho_0}(k,k)\frac{1}{s}I_s$. Since each P_{kj} has rank 1, (35) shows that

$$\widetilde{\mathbb{P}}_\rho(dk,j) \;=\; \tfrac{1}{s}\widehat{\rho_0}(k,k)dk.$$

This is a product measure and, therefore, if Y above is written as (Y_0,Z), then Y_0 and Z are independent with the stated distributions. □

Note that in Corollary 1, the definition of the quantum walk, as given by (6) and (7), affects only π, while the initial state affects only the distribution Y_0.

Remark 1. As explained at the end of Section 2, these results transfer to quantum walks on $\mathbb{Z}^d$ too. It can be verified, using the method described there, that in this case the limit distribution is described by the formulas above, but with $k \in \mathbb{K}^d$, the dual group (a d-dimensional torus). This generalizes results in [7]. In particular, if the initial position is $0 \in \mathbb{Z}^d$ with a maximally mixed coin state, Corollary 1 holds with Y_0 uniformly distributed on $\mathbb{K}^d$.

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