Weak limits for quantum random walks

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We formulate and prove a general weak limit theorem for quantum random walks in one and more dimensions. With X_n denoting position at time n, we show that X_n/n converges weakly as $n \to \infty$ to a certain distribution which is absolutely continuous and of bounded support. The proof is rigorous and makes use of Fourier transform methods. This approach simplifies and extends certain preceding derivations valid in one dimension that make use of combinatorial and path integral methods.

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I. INTRODUCTION

Let $R_1, R_2, \ldots$ be independent identically distributed random variables taking values in the reals $\mathbb{R}$, and suppose that they have common mean $\mu = E(R_1)$ and finite non-zero variance $\sigma^2 = E(R_1^2) - \mu^2$. The central limit theorem asserts that the sum $X_n = \sum_{i=1}^n R_i$ satisfies

$$\frac{X_n - n\mu}{\sigma\sqrt{n}} \Rightarrow \mathrm{N} \quad \text{as } n \to \infty \tag{1}$$

where N denotes the normal (Gaussian) distribution with mean 0 and variance 1, and $\Rightarrow$ denotes weak convergence:

$$T_n \Rightarrow T \quad \text{if} \quad E(f(T_n)) \to E(f(T)) \tag{2}$$

for all bounded continuous functions $f : \mathbb{R} \to \mathbb{R}$. An early version of this now classical theorem for random walks was proved as long ago as 1733 by de Moivre, [5]. In the modern theory, the conditions on the R_i are relaxed to allow non-independent non-identically distributed random variables taking values in general spaces. Since the weak limit of X_n, suitably normalized, depends only on the probability measures associated with the X_n, we may think of the central limit theorem as a result about weak limits of measures, rather than about the stochastic process $(X_n : n \geq 1)$ itself. This is an impoverishment of the theory, since it overlooks the random variables themselves.

There has been recent interest, [1], in a new type of process termed a quantum random walk. Quantum random walks give rise to certain sequences $(\mu_n : n \geq 1)$ of probability measures, each of which is given in terms of the preceding measures in the sequence. Whilst

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it is possible as always to construct random variables having these measures, this may not be done in a natural manner as in the theory of stochastic processes. One may nevertheless ask whether, subject to an appropriate normalization, the μ_n converge weakly to some non-trivial distributional limit. Results in this direction have been obtained for one-dimensional quantum walks by Konno [2, 3]. We show in this note how to simplify and extend such results. We introduce a new method of studying such weak limits, and we apply this method to quantum walks in one and higher dimensions.

We consider first a quantum random walk on the integers $\mathbb{Z}$. At each time n ($\in \mathbb{N}$) the state of the particle is transformed by a unitary operator described by a rotation of the internal degree of freedom followed by a conditional shift of the position, [4]; the internal degree of freedom represents a coin that determines the shift of the position. The overall state of the system belongs to the Hilbert space $H_C \otimes H_P$, where H_C is associated with the internal degree of freedom (coin space) and H_P with position. In the simplest case, we have $H_C = \mathbb{C}^2$ and $H_P = \ell^2(\mathbb{Z})$. A suitable basis for H_P is given by the eigenstates of the position operator X

$$Xv_x = xv_x, \qquad x \in \mathbb{Z}, \tag{3}$$

subject to $\langle v_x, v_{x'}\rangle = \delta_{xx'}$, the Kronecker delta. A general state of the system may be written with respect to this basis as

$$\psi = \sum_x \sum_j \psi_j(x) v_x w_j, \tag{4}$$

where the vectors w_j, $j = 1, 2$, define a standard basis in H_C. The probability $\mu_n(x)$ of finding the particle at the position x at time n is given by the standard rule

$$\mu_n(x) = \sum_j |\langle v_x\, w_j, \psi_n\rangle|^2 \tag{5}$$

where $\psi_n = U^n\psi_0$ with U the time-evolution operator of the walk and ψ_0 the initial state of the system.

The asymptotic properties of the sequence $(\mu_n : n \geq 1)$ are studied in the next section. Such results are extended in Section III to quantum walks in two and more dimensions. We highlight two special features of such asymptotics, namely: instead of normalizing by $\sqrt{n}$ as in (1), we shall normalize by n, and the weak limit is absolutely continuous with bounded support.

II. WEAK LIMIT FOR ONE-DIMENSIONAL QUANTUM WALKS

In order to define the position of a quantum particle as a random variable, we consider the evolution of the position operator in the Heisenberg picture starting from time $n = 0$. At each time n, the eigenvalues of the operator $X_n \doteq U^{\dagger n} X U^n$ define the possible values of the particle's position with corresponding probability given by (5), where the dependence on the initial state ψ_0 is explicit.

Although the position may be treated as an ordinary random variable, the sequence $(X_n : n \geq 1)$ does not define a stochastic process, since the simultaneous measurement of X_n for different n would change the quantum random walk at each step. Therefore we let the system evolve repeatedly under U up to time n, without measuring it, and then we study the properties of the distribution μ_n of X_n.

Let ψ_0 be any initial state in $H_C \otimes H_P$ with all moments $E(X^r)$ finite. In order to simplify the calculations which follow, we consider transformations in terms of wave function components, and we take the Fourier transform space $\widehat{\ell^2(\mathbb{Z})} = L^2(\mathbb{K})$, where $\mathbb{K} = [0, 2\pi)$ is thought of as the unit circle in $\mathbb{R}^2$. We define an inner product on $L^2(\mathbb{K})$ by

$$\langle \psi, \phi \rangle = \int_0^{2\pi} \overline{\psi(k)} \phi(k) \, \frac{dk}{2\pi} \tag{6}$$

and we note the isometry between $\ell^2(\mathbb{Z})$ and $L^2(\mathbb{K})$ given by

$$(\psi_x) \mapsto \sum_x \psi_x e^{ixk}, \tag{7}$$

with inverse

$$\psi \mapsto \hat{\psi} \quad \text{where} \quad \hat{\psi}(x) = \int_0^{2\pi} e^{-ixk} \psi(k) \, \frac{dk}{2\pi}. \tag{8}$$

The right shift S on $\ell^2(\mathbb{Z})$ given by $S(\psi_x)_{-\infty}^{\infty} = (\psi_{x-1})_{-\infty}^{\infty}$ corresponds to the multiplication operator $\hat{S}\psi = e^{ik}\psi$ on $L^2(\mathbb{K})$.

Our fundamental Hilbert space is thus $H = H_C \otimes L^2(\mathbb{K})$, the space of $\mathbb{C}^2$-valued functions

$$\psi(k) = \begin{pmatrix} \psi_1(k) \\ \psi_2(k) \end{pmatrix} \tag{9}$$

on $\mathbb{K}$ satisfying

$$\|\psi\|^2 = \|\psi_1\|_{L^2}^2 + \|\psi_2\|_{L^2}^2 < \infty.$$

As usual, we consider state vectors normalized by $\|\psi\|^2 = 1$. The evolution of the walk comprises repeated applications of an internal transformation (coin toss) A acting on $\mathbb{C}^2$, followed by the shift S given by

$$S \begin{pmatrix} \psi_1(k) \\ \psi_2(k) \end{pmatrix} = \begin{pmatrix} e^{ik}\psi_1(k) \\ e^{-ik}\psi_2(k) \end{pmatrix}. \tag{10}$$

Thus the total evolution U on H is given by

$$U\psi = \begin{pmatrix} e^{ik} & 0 \\ 0 & e^{-ik} \end{pmatrix} A \begin{pmatrix} \psi_1(k) \\ \psi_2(k) \end{pmatrix} = U(k)\psi(k). \tag{11}$$

If we begin the quantum random walk with an initial state $\Psi_0 \in H$, its state after n steps is

$$\Psi_n = U^n \Psi_0 = U(k)^n \Psi_0(k). \tag{12}$$

For each k, $U(k)$ has two eigenvalues $\lambda_1(k)$ and $\lambda_2(k)$ with $|\lambda_j(k)| = 1$, and has corresponding eigenvectors $v_1(k)$, $v_2(k) \in \mathbb{C}^2$ that define a basis for H. We assume henceforth that

$$\lambda_1(k) \neq \lambda_2(k), \tag{13}$$

since otherwise $U(k)$ is diagonal; by (11) then A is diagonal and the state evolves trivially, either to the right or to the left.

The mapping $k \mapsto U(k)$ is C^∞ and the eigenvalues are distinct for each k, and therefore the eigenvalues $\lambda_j(k)$ are C^∞ functions of k, and the eigenvectors $v_j(k)$ may be chosen to be C^∞ with normalization $\|v_j(k)\| = 1$. By expanding the wave function in terms of this basis, the nth time evolution becomes

$$\Psi_n(k) = U(k)^n \Psi_0(k) = \lambda_1(k)^n \langle v_1(k), \Psi_0(k)\rangle v_1(k) + \lambda_2(k)^n \langle v_2(k), \Psi_0(k)\rangle v_2(k), \tag{14}$$

where each component on the right hand side is a C^∞ function of k. The moments of the position distribution are given in terms of the operator X according to the standard formula

$$E\left(X_n^r\right) = \langle \Psi_n, X^r \Psi_n\rangle. \tag{15}$$

Using the isometry between $\ell^2(\mathbb{Z})$ and $L^2(\mathbb{K})$, the above expectation may be written as

$$E\left(X_n^r\right) = \int_0^{2\pi} \langle \Psi_n(k), D^r \Psi_n(k)\rangle \frac{dk}{2\pi}, \tag{16}$$

where $D = \hat{X} = -id/dk$ is the position operator in the momentum space $L^2(\mathbb{K})$. For fixed r we can compute $D^r\Psi_n(k)$ by (14) and Leibniz' rule. It is easily seen that

$$D^r \Psi_n(k) = \sum_j (n)_r \lambda_j(k)^{n-r} (D\lambda_j(k))^r \langle v_j(k), \Psi_0(k)\rangle v_j(k) + \mathrm{O}(n^{r-1}), \tag{17}$$

where $(n)_r = n(n-1)\cdots(n-r+1)$. Equations (16) and (17) yield, as $n \to \infty$,

$$\begin{aligned} E[(X_n/n)^r] &= \int_0^{2\pi} \sum_j \lambda_j(k)^{n-r} \left(D\lambda_j(k)\right)^r \langle v_j(k), \Psi_0(k)\rangle \langle \Psi_n(k), v_j(k)\rangle \frac{dk}{2\pi} + \mathrm{O}(n^{-1}) \\ &= \int_0^{2\pi} \sum_j \left(\frac{D\lambda_j(k)}{\lambda_j(k)}\right)^r |\langle v_j(k), \Psi_0(k)\rangle|^2 \frac{dk}{2\pi} + \mathrm{O}(n^{-1}). \end{aligned} \tag{18}$$

Let $\Omega = \mathbb{K} \times \{1,2\}$, let μ be the probability measure on Ω given by $|\langle \Psi_0(k), v_j(k)\rangle|^2 dk/2\pi$ on $\mathbb{K} \times \{j\}$. Let $h_j(k) = \lambda_j(k)^{-1} D\lambda_j(k)$ and define $h : \Omega \to \mathbb{R}$ by $h(k,j) = h_j(k)$. (h is real because $|\lambda_j(k)| = 1$.) By (18),

$$E[(X_n/n)^r] \to \int_\Omega h^r \, d\mu \quad \text{as } n \to \infty. \tag{19}$$

Since h is bounded and the above relation holds for all integers $r \geq 0$, we deduce by the method of moments the following. (See [6] for the general theory of weak convergence.)

Theorem 1. *With notation as above,*

$$\frac{1}{n} X_n \Rightarrow Y = h(Z) \quad \textit{as } n \to \infty, \tag{20}$$

where Z is a random element of Ω with distribution μ.

In particular, the support of Y is $[\min h, \max h]$, the range of h, at least provided the density of μ given above does not vanish on some interval.

A similar weak limit theorem for X_n/n has been proved by Konno [2, 3], by different methods and with a quite different description of the limit.

We note that no assumption has been made above on the matrix A and the initial state ψ_0, and thus the above result holds for any unitary quantum walk on the integers, subject only to (13). Note also that μ depends only on the overlap between the initial state of the system and the eigenvectors of $U(k)$, whereas h depends only on the coin flip matrix A.

As an example, we consider some specific cases of unitary quantum walks. We consider first the Hadamard matrix

$$A = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \tag{21}$$

By simple calculus,

$$\lambda_j(k) = \frac{i}{\sqrt{2}} \sin k \pm \sqrt{1 - \tfrac{1}{2} \sin^2 k} \tag{22}$$

and thus

$$h(k,j) = \frac{-i\lambda_j'(k)}{\lambda_j(k)} = \pm \frac{\cos k}{\sqrt{2 - \sin^2 k}}. \tag{23}$$

Hence the limit distribution is concentrated on the interval

$$[\min h, \max h] = \left[-\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}} \right]. \tag{24}$$

For a general unbiased walk, we take as coin flip the unitary matrix

$$U(\varphi, \psi) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i(\varphi+\psi)} & e^{-i(\varphi-\psi)} \\ e^{i(\varphi-\psi)} & -e^{-i(\varphi+\psi)} \end{pmatrix}, \tag{25}$$

where $\varphi, \psi \in \mathbb{R}$, with corresponding evolution

$$U(k) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{ik} e^{i(\varphi+\psi)} & e^{ik} e^{-i(\varphi-\psi)} \\ e^{-ik} e^{i(\varphi-\psi)} & -e^{-ik} e^{-i(\varphi+\psi)} \end{pmatrix} \doteq U_{\varphi\psi}(k). \tag{26}$$

With $\varphi + \psi = a$, $\varphi - \psi = b$, the eigenvalues may be written in the form

$$\lambda_j(k) = \frac{i}{\sqrt{2}} \sin(k+a) \pm \sqrt{1 - \tfrac{1}{2} \sin^2(k+a)}, \tag{27}$$

and therefore

$$h(k,j) = \frac{-i\lambda_j'(k)}{\lambda_j(k)} = \pm \frac{\cos(k+a)}{\sqrt{2 - \sin^2(k+a)}}. \tag{28}$$

Thus the general unbiased walk has exactly the same behaviour as the Hadamard case, subject to a shift in the momentum parameter of the wave amplitudes. We have as before that the domain of the limit distribution is as in (24).

Finally we introduce a "biased" random walk by defining a *bias factor* ρ in the coin flip matrix

$$U(\rho) = \begin{pmatrix} \sqrt{\rho} & \sqrt{1-\rho} \\ \sqrt{1-\rho} & -\sqrt{\rho} \end{pmatrix}, \tag{29}$$

that gives rise to the evolution

$$U_\rho(k) = \begin{pmatrix} e^{ik}\sqrt{\rho} & e^{ik}\sqrt{1-\rho} \\ e^{-ik}\sqrt{1-\rho} & -e^{-ik}\sqrt{\rho} \end{pmatrix}. \tag{30}$$

The evolution under U of a general two-component wave-function corresponds to

$$\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \mapsto \begin{pmatrix} e^{ik} & 0 \\ 0 & e^{-ik} \end{pmatrix} \begin{pmatrix} \sqrt{\rho}\psi_1(k) + \sqrt{1-\rho}\psi_2(k) \\ \sqrt{1-\rho}\psi_1(k) + \sqrt{\rho}\psi_2(k) \end{pmatrix}, \tag{31}$$

where the two internal states transform differently. In fact, the first component receives a kick of momentum $+k$ with probability ρ and $-k$ with probability $1-\rho$; the opposite holds for the second component.

In terms of ρ, the eigenvalues are

$$\lambda_j(k) = i\sqrt{\rho}\sin k \pm \sqrt{1-\rho\sin^2 k} \tag{32}$$

and thus

$$h(k,j) = \frac{-i\lambda_j'(k)}{\lambda_j(k)} = \pm\frac{\cos k}{\sqrt{\rho^{-1}-\sin^2 k}}. \tag{33}$$

It follows that $[\min h, \max h] = [-\sqrt{\rho}, \sqrt{\rho}]$, whence the bias factor of the walk sets a limit on the asymptotic momentum distribution by changing the support of the limit distribution.

The representation (20) of the limit variable allows a direct computation of the asymptotic probability density function in most cases of interest. For example, assume that the initial state is at position 0. If the coin initially is in a given state $i = 1$ or 2, then $\Psi_0(k) = \binom{1}{0}$ or $\binom{0}{1}$, respectively, and thus $\mu = |v_{ji}(k)|^2\, dk/2\pi$ on $\mathbb{K} \times \{j\}$. If we consider instead a random initial state of the coin, we have a mixture of these two pure states and thus

$$\mu = \frac{1}{2}\sum_{i=1}^{2} |v_{ji}(k)|^2 \frac{dk}{2\pi} = \frac{dk}{4\pi} \tag{34}$$

on $\mathbb{K} \times \{j\}$; that is, μ is the uniform distribution on Ω. In the Hadamard case, for example, with h given by (23), if $X_0 = 0$ and the coin initially random, then, for $-1/\sqrt{2} \le y \le 1/\sqrt{2}$,

$$\begin{aligned} P(Y \le y) &= \int_{h^{-1}([-\infty,y])} d\mu \\ &= 2\int_{\cos k/\sqrt{1+\cos^2 k}\le y} \frac{dk}{4\pi} \\ &= 1 - \frac{1}{\pi}\arccos\left(\frac{k}{\sqrt{1-k^2}}\right), \end{aligned}$$

which gives as density $f(y)$ of Y,

$$f(y) = \frac{dy}{\pi(1-y^2)\sqrt{1-2y^2}}, \tag{35}$$

in agreement with the result of [2]. The same holds for every unbiased walk defined by (25).

The above result can be interpreted as the weak convergence of the sequence $\hat{X}_n/n$ of operators on H, as $n \to \infty$, to an operator V, defined on a dense subspace of H with spectral resolution

$$V = \int \sum_j \left(\frac{D\lambda_j(k)}{\lambda_j(k)}\right) dE_j(k), \tag{36}$$

where $dE_j(k)$ is the projector over the eigenspace corresponding to the eigenvalue $\lambda_j(k)$ of $U(k)$. (The weak convergence of unbounded operators here is formally defined as the weak convergence of the corresponding unitary operators $\exp(is\hat{X}_n/n) \to \exp(isV)$ for every real s.) The limit operator is diagonal in the eigenbasis of the unitary evolution of the walk and gives

$$\langle \hat{X}_n \rangle \sim \langle V \rangle n, \tag{37}$$

that represents the Heisenberg equation of motion for the position, in the limit $n \to \infty$, if we interpret V as the "velocity" operator. Thus, asymptotically, the centre of the wave packet moves with constant speed, given by V. It is worth pointing out that, although the equation of motion resembles the one of a classical system with constant velocity, the state of the quantum particle spreads in time, with a quadratic growth in the variance of the position distribution.

III. WEAK LIMIT FOR d-DIMENSIONAL QUANTUM WALKS

Let $d \geq 1$. The classical random walk on the integer lattice $\mathbb{Z}^d$ models the motion of a particle that moves in an unbiased manner in a d-dimensional space. Let $\mathbf{e}_i$, $i \in \{1, 2, \ldots, n\}$, be the unit vector in the direction of increasing ith coordinate. Let $\mathbf{R}_1, \mathbf{R}_2, \ldots$ be independent identically distributed random variables, each being uniform on the set $\{\pm\mathbf{e}_i : i = 1, 2, \ldots, d\}$. The position of the particle at time n is given as the sum

$$\mathbf{X}_n = \sum_{j=1}^{n} \mathbf{R}_j. \tag{38}$$

By the central limit theorem for d-dimensional random walk, the random vector $\mathbf{X}_n/\sqrt{n}$ converges weakly as $n \to \infty$ to a random vector in $\mathbb{R}^d$ having the multivariate normal distribution $N(0, I/d)$, where I is the $d \times d$ identity matrix. We shall see in the following that a corresponding weak convergence holds for a d-dimensional quantum random walk.

The 1-dimensional quantum random walk of the last section may be extended to d dimensions as follows. Let $\boldsymbol{\epsilon}_1, \ldots, \boldsymbol{\epsilon}_{2d}$ denote the $2d$ possible shift vectors $\pm\mathbf{e}_i$, $i = 1, 2, \ldots, d$. The state of the system is a vector $\Psi = (\Psi(\mathbf{k})_J)_{J=1}^{2d} \in H = L^2(\mathbb{K}^d) \otimes \mathbb{C}^{2d}$ where $\mathbf{k} = (k_1, k_2, \ldots, k_d)$ and the Jth component corresponds to a shift by the vector $\boldsymbol{\epsilon}_J$. At each time, the state is transformed by applying a rotation A acting on $\mathbb{C}^{2d}$, followed by a d-dimensional shift on $L^2(\mathbb{K}^d)$, cf. (10),

$$S^{(d)}\Psi(\mathbf{k})_J = e^{i\boldsymbol{\epsilon}_J \cdot \mathbf{k}} \Psi(\mathbf{k})_J. \tag{39}$$

The general unitary operator that evolves the walk from time $n = 0$ is thus

$$U(\mathbf{k}) = \mathcal{D}\{e^{i\boldsymbol{\epsilon}_1 \cdot \mathbf{k}}, \ldots, e^{i\boldsymbol{\epsilon}_{2d} \cdot \mathbf{k}}\} A, \tag{40}$$

where $\mathcal{D}$ denotes the $2d$ diagonal matrix. The operator $U(\mathbf{k})$ can be diagonalized in H, and has $2d$ eigenvalues and $2d$ eigenvectors. Assume that one may choose the latter as C^∞ functions of $\mathbf{k}$. (See the remark at the end of the section.) Let $v_J(\mathbf{k})$, $\lambda_J(\mathbf{k})$ be respectively the eigenvectors and eigenvalues of $U(\mathbf{k})$, with $J = 1, 2, \ldots, 2d$. The initial state of the system can be written in this basis as

$$\Psi_0(\mathbf{k}) = \sum_{J=1}^{2d} \langle v_J(\mathbf{k}), \Psi_0(\mathbf{k}) \rangle v_J(\mathbf{k}) \tag{41}$$

and the state at time n as

$$\Psi_n(\mathbf{k}) = \sum_{J=1}^{2d} \lambda_J^n(\mathbf{k}) \langle v_J(\mathbf{k}), \Psi_0(\mathbf{k})\rangle v_J(\mathbf{k}). \tag{42}$$

The d-dimensional position operator $X^{(d)} = (X_1, X_2, \ldots, X_d)$ acts on $L^2(\mathbb{K}^d)$ as the differential vector operator $D^{(d)} = (-id/dk_1, -id/dk_2, \ldots, -id/dk_d)$. By considering each component of $D^{(d)}$ separately, it is easily seen that the operators $\hat{X}_{i,n}$ converge weakly on H, as $n \to \infty$, to the corresponding components V_i, where

$$V_i = \int \sum_J \left(\frac{D_i \lambda_J(\mathbf{k})}{\lambda_J(\mathbf{k})} \right) dE_J(\mathbf{k}), \tag{43}$$

where $dE_J(\mathbf{k})$ denotes again the projector onto the eigenspace of $U(\mathbf{k})$ with eigenvalue $\lambda_J(\mathbf{k})$. This does not imply, however, that the sequence of random vectors associated with the process converges weakly on $\Omega = \mathbb{K}^d \times \{1, \ldots, 2d\}$. In general, the evolution operator $U(\mathbf{k})$ generates entanglement between the different spatial directions and it is necessary therefore to consider also the correlation terms between different components of $\hat{X}^{(d)}$.

The so-called Cramér–Wold device enables a simplification: in order that a sequence of random variables converge weakly, it suffices that all linear combinations converge. More properly, we have the following, see [6], Theorem 29.4.

Theorem 2. *Consider a sequence* $\mathbf{X}_n = (X_{1,n}, X_{2,n}, \ldots, X_{d,n})$*,* $n \geq 1$*, of random d-vectors, and let* $\mathbf{Y} = (Y_1, Y_2, \ldots, Y_d)$ *be a random d-vector. If*

$$\sum_{j=1}^{d} c_j X_{j,n} \Rightarrow \sum_{j=1}^{d} c_j Y_j \quad \text{as } n \to \infty, \tag{44}$$

for all $\mathbf{c} = (c_1, c_2, \ldots, c_d) \in \mathbb{R}^d$*, then* $\mathbf{X}_n \Rightarrow \mathbf{Y}$.

Suppose for simplicity that $d = 2$. For fixed r, we compute the expectation

$$E\left[\left(\sum_{j=1}^{2} c_j \hat{X}_{j,n}/n \right)^r \right] = \frac{1}{n^r} \sum_{p=0}^{r} \binom{r}{p} c_1^{r-p}\, c_2^p \,\langle \Psi_n, D_1^{r-p}\, D_2^p\, \Psi_n \rangle, \tag{45}$$

where we have used the fact that operators along different directions commute. We have

$$D_2^p \Psi_n(\mathbf{k}) = \sum_J (n)_p \lambda_J^{n-p}(\mathbf{k})\, (D_2 \lambda_J(\mathbf{k}))^p \;\langle v_J(\mathbf{k}), \Psi_0(\mathbf{k})\rangle v_J(\mathbf{k}) + \mathrm{O}(n^{p-1}) \tag{46}$$

$$D_1^{r-p}[D_2^p \Psi_n(\mathbf{k})] = \sum_J (n)_r \lambda_J^{n-r}(\mathbf{k})\, (D_1 \lambda_J(\mathbf{k}))^{r-p}\, (D_2 \lambda_J(\mathbf{k}))^p \;\langle v_J(\mathbf{k}), \Psi_0(\mathbf{k})\rangle v_J(\mathbf{k}) + \mathrm{O}(n^{r-1}). \tag{47}$$

Thus, as $n \to \infty$,

$$
\begin{aligned}
& E\left[\left(\frac{(c_1\hat{X}_1 + c_2\hat{X}_2)_n}{n}\right)^r\right] \\
& \quad \to \int \sum_J \left\{ \sum_{p=0}^r \binom{r}{p} c_1^{r-p}\, c_2^p\, h_1(\mathbf{k}, J)^{r-p} h_2(\mathbf{k}, J)^p \right\} |\langle v_J(\mathbf{k}), \Psi_0(\mathbf{k})\rangle|^2 \frac{d\mathbf{k}}{(2\pi)^2} \\
& \quad = \int \sum \{c_1 h_1(\mathbf{k}, J) + c_2 h_2(\mathbf{k}, J)\}^r\, |\langle v_J(\mathbf{k}), \Psi_0(\mathbf{k})\rangle|^2 \frac{d\mathbf{k}}{(2\pi)^2},
\end{aligned}
$$

where $h_i(\mathbf{k}, J) = \lambda_J(\mathbf{k})^{-1} D_i \lambda_J(\mathbf{k})$, $i = 1, 2$. With $\Omega = \mathbb{K}^2 \times \{1, 2, 3, 4\}$, and $Z_n = c_1 X_{1,n} + c_2 X_{2,n}$, we have

$$
E\left[(Z_n/n)^r\right] \to \int_\Omega (c_1 h_1 + c_2 h_2)^r \, d\mu, \tag{48}
$$

where μ is the probability measure on Ω given by

$$
d\mu = |\langle v_J(\mathbf{k}), \Psi_0(\mathbf{k})\rangle|^2 \frac{d\mathbf{k}}{(2\pi)^2} \quad \text{on } \mathbb{K}^2 \times \{J\}. \tag{49}
$$

By the method of moments as in the one-dimensional case and the Cramér–Wold device (Theorem 2), we obtain a generalization of Theorem 1 to the two-dimensional case.

As a simple example, consider the two-dimensional generalization of the Hadamard matrix given by

$$
A = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix}. \tag{50}
$$

In the above notation, the unitary operator that evolves the walk is represented by

$$
U(\mathbf{k}) = \mathcal{D}\{e^{ik_1}, e^{ik_2}, e^{-ik_2}, e^{-ik_1}\} A. \tag{51}
$$

The operator $U(\mathbf{k})$ may be expressed thus as a tensor product of two one-dimensional operators that describe Hadamard walks along the directions defined by $k^+ = (k_1 + k_2)/2$ and $k^- = (k_1 - k_2)/2$:

$$
U(\mathbf{k}) = U(k^+) \otimes U(k^-). \tag{52}
$$

Its eigenvalues and eigenvectors are products of those of $U(k^+)$, $U(k^-)$ respectively, and therefore

$$
\lambda_J(\mathbf{k}) = \lambda_{j_+}(k^+)\, \lambda_{j_-}(k^-), \tag{53}
$$

where the λ_j, $j = 1, 2$, are given by (22) and $J = 1, 2, 3, 4$ labels the pairs (j_+, j_-) in some order. Thus

$$
h_i(\mathbf{k}, J) = \lambda_J(\mathbf{k})^{-1} D_i \lambda_J(\mathbf{k}) = \pm \frac{\cos(k^+)}{2\sqrt{2 - \sin^2(k^+)}} \pm (-1)^{i-1} \frac{\cos(k^-)}{2\sqrt{2 - \sin^2(k^-)}}. \tag{54}
$$

for $i = 1, 2$. The limit velocity operator $\mathbf{V}$ is given by $\mathbf{V} = (V_1, V_2)$, with

$$
V_i = \int \sum_J h_i(\mathbf{k}, J)\, dE_J(\mathbf{k}), \quad J = 1, 2, 3, 4. \tag{55}
$$

The result may be extended to arbitrary dimension $d \geq 2$ using the same argument, yielding the following result.

Theorem 3. *For the d-dimensional quantum random walk,*

$$\frac{1}{n}\mathbf{X}_n \Rightarrow \mathbf{Y} = \big(h_1(Z), \dots, h_d(Z)\big), \tag{56}$$

where Z is a random element of $\Omega = \mathbb{K}^2 \times \{1, \dots, 2d\}$ with distribution μ given by (49) *and $h_i(\mathbf{k}, J) = \lambda_J(\mathbf{k})^{-1} D_i \lambda_J(\mathbf{k})$.*

The limit observable is again diagonal in the eigenbasis of $U(\mathbf{k})$ and represents the velocity for $n \to \infty$.

Technical remark. We assumed above that the eigenvectors of $U(\mathbf{k})$ can be chosen as C^∞ functions of $\mathbf{k}$. We do not know if this is always possible when $d \geq 2$, but it can be replaced by the following, weaker hypothesis, which we believe always holds: There exists an open subset O of $\mathbb{K}^d$ with full Lebesgue measure (that is, the complement is a null set) such that the eigenvectors (and thus the eigenvalues) can be chosen infinitely differentiable in O. (For example, this holds if there is any point $\mathbf{k}$ where $U(\mathbf{k})$ has distinct eigenvalues, because we then can choose O as the subset of $(0, 2\pi)^d$ where the discriminant is non-zero; we omit the proof that this set has the required properties.)

Under this assumption, the argument above holds for every initial value that is an infinitely differentiable function with support in O. (The function h will be defined on $O \times \{1, 2, \dots, 2d\}$, but that is enough.) Such functions are dense in H, by a standard L^2 result. Hence, given any initial state Ψ_0, and an $\epsilon > 0$, we can find an initial state Ψ_0^ϵ with $\|\Psi_0 - \Psi_0^\epsilon\| < \epsilon$ for which

$$\frac{1}{n}\mathbf{X}_n^\epsilon \Rightarrow \big(h_1(Z^\epsilon), \dots, h_d(Z^\epsilon)\big). \tag{57}$$

Since the evolution operators are unitary, we have $\|\Psi_n - \Psi_n^\epsilon\| = \|\Psi_0 - \Psi_0^\epsilon\| < \epsilon$ for every n, and it follows that for any observable event A, the probabilities $\mathbb{P}(\mathbf{X}_n \in A)$ and $\mathbb{P}(\mathbf{X}_n^\epsilon \in A)$ differ by at most 2ϵ. Similarly, it is easy to see from (49) that $|\mathbb{P}(Z \in B) - \mathbb{P}(Z^\epsilon \in B)| < 2\epsilon$ for every $B \subset \Omega$. It is now easy to interchange the two limits $\epsilon \to 0$ and $n \to \infty$ and obtain (56); see [6], Theorem 4.2. Theorem 3 thus holds for every initial state, also under the weaker assumption.

IV. FURTHER EXTENSIONS

We have, for simplicity, only considered simple random walks, where the shifts are by unit vectors. More generally, we can allow shifts by any given finite set $\{\boldsymbol{\epsilon}_1, \boldsymbol{\epsilon}_2, \dots, \boldsymbol{\epsilon}_N\}$ of vectors in $\mathbb{Z}^d$. The coin flip is now represented by a unitary matrix A in $\mathbb{C}^N$. Theorem 3 extends to this case, with $2d$ replaced by N, by the same proof.

An interesting example is when the shift vectors are the 2^d vectors in $\{-1, 1\}^d$; thus each coordinate is shifted by ± 1 in each step.

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