The Random Walk in Generalized Quantum Theory*

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Abstract

One can view quantum mechanics as a generalization of classical probability theory that provides for pairwise interference among alternatives. Adopting this perspective, we "quantize" the classical random walk by finding, subject to a certain condition of "strong positivity", the most general Markovian, translationally invariant "decoherence functional" with nearest neighbor transitions.

1 Introduction

In the causal set approach to quantum gravity [1] the basic entity is taken to be a discrete causal order. This, to our knowledge, is the only candidate theory of quantum gravity, that naturally predicts a cosmological constant of the right magnitude. (The predicted cosmological constant is related inversely to the square root of the total number of spacetime elements in the universe, there being roughly one element per Planck volume, [2].) On a classical level, one has a well defined stochastic dynamical scheme for causets, and much is understood about this "CSG" model,[1] especially about its special case of "transitive percolation" [3, 4, 5, 6, 7]. Although interesting and instructive in its own right, this model was intended first of all as a stepping stone to quantum gravity, which in this context would be a quantum dynamics related to the CSG model analogously to how the quantum dynamics of a free particle is related to the classical stochastic process of diffusion ("Wiener process"). However, given the finitary nature of the causal set, it seems unlikely that such a quantum process could be unitary, and it is natural to look for a wider setting in which a suitable dynamics might be found.

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[1] The initials stand for "classical sequential growth".

Quantum measure theory (see below) offers such a setting, and our primary goal in the present paper is to explore the analog of the classical random walk in this setting. More specifically, we will be interested in Markov processes with nearest neighbor transitions. This problem seems particularly apt as a "warm up" for causal sets, because, here also, the discreteness of the random walk obstructs a unitary "quantization" of the classical stochastic process.[2] In this way, the discrete case differs markedly from the continuous one: the diffusion equation in the continuum has a unitary analog in the Schrödinger equation, whereas the random walk on the integers has, strictly speaking, no unitary analog at all.

A second reason for interest in the quantal[3] random walk comes not from quantum gravity at its fundamental level, but from a recent phenomenological theory which attempts to implement in a concrete model the aforementioned suggestion from causal set theory that the cosmological constant Λ would be subject to $1/\sqrt{N}$ fluctuations. This phenomenological theory [10] introduces a (classical) random walk to act as the source of the fluctuations, but it would seem more logical for the source to be quantum in nature, since the fluctuations are supposed to be rooted in an analog of the time-energy uncertainty principle. In other words, it would be natural to use a quantum random walk as the source of the fluctuations, but first one should know what a quantum random walk is!

Thirdly, we believe that, independent of any application to quantum gravity, the problem of the quantum random walk is of interest in itself, as perhaps the simplest example of a situation where one is forced to the type of generalization of unitary quantum mechanics called "generalized quantum mechanics" in [11] and "quantum measure theory" in [12, 13]. Moreover, natural questions arise in this connection which seem not to have been addressed so far, for example the question whether there exists a quantum analog of the central limit theorem, which classically almost guarantees the existence of a unique continuum limit. If there does exist such a limit, one would expect it to be the "Schrödinger process", i.e. the "quantum stochastic process" corresponding to the Schrödinger equation. But whether or not some sort of central limit theorem obtains, one can still ask whether any quantum random walk has the Schrödinger process as its limit. To our knowledge, this question remains open (cf. [8, 9]), but one might hope to settle it using the techniques we develop herein. Indeed, we hope that one of the processes we construct below will have the desired limit. Among other things, this would illustrate how a non-unitary discrete process can become unitary in a continuum limit (and this in turn would be of great interest for quantum gravity).

As just intimated, we will seek a theory of the quantal random walk formulated as a generalized measure theory [12, 13, 11, 14, 15]. When thought of in this way, quantum mechanics is seen to reside in level 2 of an infinite hierarchy of generalized measures, graded by the degree of interference they allow for (with pairwise interference being characteristic of the quantum level). Let us briefly review this framework.

Classical probability theory assigns a probability $P(A)$ to a subset A of the set of all "con-

[2] More precisely, no nontrivial unitary process exists which is Markovian and for which the random walker carries no internal variables and makes only nearest neighbor transitions [8]. By allowing a one-step memory, or equivalently, endowing the walker with a two-valued internal state, one can salvage unitarity, and several models of this sort have been discussed in the literature [8, 9].

[3] Quantal will be used to refer to the generalised quantum measure theories studied in this paper, of which unitary quantum mechanics is only one particular case.

figurations",[4] and such probabilities satisfy the familiar Kolmogorov sum rule:

$$P(A \sqcup B) = P(A) + P(B) \tag{1}$$

where $A \sqcup B$ is the disjoint union of A and B. This sum rule yields measure-theory in the classical sense, and, physically, it is appropriate for the description of classical stochastic processes such as Brownian motion. But the additivity of classical probabilities is only the first, and most restrictive, in a hierarchy of possible sum-rules, each of which implies its successor.

The next weaker sum-rule defines a *generalized measure theory* which includes quantum mechanics as a special case. We will refer to a generalized measure satisfying this sum-rule as a "quantum" or "quantal" measure and a physical process described by such a measure as a quantal process or a generalized quantum process. The fact that quantum probabilities can be expressed "as the squares of amplitudes" is a natural consequence of this sum rule. Even weaker sum-rules provide further generalizations of classical probability theory that we will now define, but without then considering them any further.

In its quantal measure formulation, the familiar quantum mechanics of point-particles does its job by furnishing "generalized probabilities" for sets of trajectories. More formally, it associates to a set A of trajectories a non-negative real number denoted $\mu(A)$ or $|A|$ which is called its *quantal measure*; and it is this measure that enters into the sum-rules. The deviation from the classical case consists in the fact that the *interference term*

$$I(A, B) := |A \sqcup B| - |A| - |B|$$

between two disjoint sets of trajectories A and B is in general not zero.

Consider the following generalizations of this interference term.

$$\begin{aligned} I_1(A) &\equiv |A| & (2)\\ I_2(A,B) &\equiv |A \sqcup B| - |A| - |B| & (3)\\ I_3(A,B,C) &\equiv |A \sqcup B \sqcup C| - |A \sqcup B| - |B \sqcup C| - |A \sqcup C| + |A| + |B| + |C|, & (4) \end{aligned}$$

or in general,

$$I_n(A_1, A_2, \cdots, A_n) \equiv |A_1 \sqcup A_2 \sqcup \cdots A_n| - \sum |\bigsqcup_{j=1}^{n-1} A_{\sigma_j}| + \sum |\bigsqcup_{j=1}^{n-2} A_{\sigma_j}| - \cdots \pm \sum_{j=1}^{n} |A_j|, \tag{5}$$

where all the sets A_i are mutually disjoint and σ indexes the subsets of $\{1, 2, \cdots, n\}$ with the appropriate cardinality.

These expressions are related serially by the identity

$$I_{n+1}(A_0, A_1, A_2, \cdots, A_n) = I_n(A_0 \sqcup A_1, A_2, \cdots, A_n) - I_n(A_0, A_2, \cdots, A_n) - I_n(A_1, A_2, \cdots, A_n) \tag{6}$$

So, for each n one obtains a possible sum-rule by setting I_n to zero, and one sees that if the n^{th} such sum-rule is satisfied, then the $(n+1)^{st}$ is automatically also satisfied. Hence the sum-rules form a hierarchy of ever decreasing strength. The first sum-rule in the hierarchy,

[4] In general the configurations can be anything, but in the context of this paper they will comprise the possible trajectories of a random walker.

$I_1 = 0$, trivializes the measure and is therefore uninteresting. The second expresses precisely the additivity of classical measure theory, or equivalently the additivity of classical probabilities, when they are regarded as set-functions in the Kolmogorov manner. Accordingly, the third sum-rule, $I_3(A, B, C) \equiv 0$, defines a generalization of measure theory which, although it allows for pairwise interference of alternatives, still preserves most of the additivity of classical probabilities. This is the level of quantal measure theory.[5] The fourth and higher sum-rules define still more general forms of measure theory which may be regarded as natural extensions of quantum mechanics, and which incoroporate interference among successively larger numbers of alternatives.

Plainly, the interference term is totally symmetric in its arguments, and thus I_{n+1} vanishes if and only if I_n is "additive" in each argument, given their mutual disjointness. Thus each sum-rule is associated with a kind of multilinearity (or rather multi-additivity) of the function which measures the failure of the next stronger sum-rule to hold. At the quantum level, specifically, we learn that I_2 is bi-additive, and the peculiar quadratic relationship between quantum amplitudes and probabilities corresponds directly to this feature of I_2. In the current work we limit ourselves to the quantal case as defined by the $n = 3$ sum-rule,

$$|A \sqcup B \sqcup C| - |A \sqcup B| - |B \sqcup C| - |A \sqcup C| + |A| + |B| + |C| = 0. \tag{7}$$

Given this sum-rule, we have that I_2, which we will subsequently denote by I is bi-additive in the sense that

$$I(A \sqcup B, C) = I(A, C) + I(B, C), \tag{8}$$

whenever A, B and C are mutually disjoint. Taking

$$I(X, X) \equiv 2\,|X|. \tag{9}$$

as the value of I on equal arguments, we can extend the above definitions to arbitrary arguments, and in fact the value of I is completely determined by bi-additivity and can be given in terms of the quantal measure in, for example, either of the following equivalent forms [12]:

$$\begin{aligned} I(A, B) &= |A \cup B| + |A \cap B| - |A \backslash B| - |B \backslash A|, \\ I(A, B) &= |A \Delta B| + |A| + |B| - 2\,|A \backslash B| - 2\,|B \backslash A|. \end{aligned} \tag{10}$$

In these equations the symbol '\' denotes set-theoretic difference and 'Δ' denotes symmetric difference.

Note that any generalized measure obeying the quantum sum rule $I_3 = 0$ can be expressed in the form $|X| = I(X, X)/2$, where I is the bi-additive, real-valued set function of (10). Conversely, we could begin with such a set-function whose diagonal values are all non-negative, and use it to define a quantal measure $|\cdot|$ obeying the sum rule (7).

In unitary quantum mechanics (pretending that the set of all possible particle paths has finite cardinality) the measure of any set $A = \{x, y, \cdots, z\}$ of paths can be expressed formally

[5] In addition to this sum rule, what is called quantum measure theory in [13] is characterized by the axiom that no set of measure zero can interfere with any other (disjoint) set: $|A \sqcup N| = |A|$ for all N such that $|N| = 0$. This will follow trivially from "strong positivity", as shown in Theorem 2.

as $|A| =$ "$(1/2)I(x+y+\cdots z, x+y+\cdots z)$", which is to be evaluated by expanding out the sums via bilinearity and interpreting $I(x,y)$ as $I(\{x\},\{y\})$ with

$$I(\{x\},\{y\}) = \delta(x(T),y(T))\, e^{iS(x)}e^{-iS(y)} + (\text{complex conjugate}), \tag{11}$$

where T is a "truncation time" lying to the future of the properties defining A, and x and y are truncated paths with final end points at time T (see [16] for more details). A striking feature of unitary quantum mechanics from this point of view is the presence in $I(x,y)$ of a delta-function which "ties together" the endpoints created by truncating the paths.

A glance at this last equation reveals that $I(A,B)$ is twice the real part of the so called *decoherence functional* $D(A,B)$ where

$$D(x,y) = \delta(x(T),y(T))\, e^{iS(x)}e^{-iS(y)}. \tag{12}$$

Notice that $D(x,y)$ exhibits the symmetry property of a hermitian matrix:

$$D(y,x) = D^*(x,y). \tag{13}$$

For our purposes, the decoherence functional can be taken to be the more primitive object, since the Markov property we wish to implement is naturally expressed in terms of D but not I or the generalized measure μ itself. A decoherence functional specifying a quantal measure (i.e. a level two generalized measure) will be required to satisfy:

i) bi-additivity,

$$D(A \sqcup B, C) = D(A,C) + D(B,C) \quad \text{and} \quad D(A, B \sqcup C) = D(A,B) + D(A,C), \tag{14}$$

ii) hermiticity

$$D(A,B) = D^*(B,A), \tag{15}$$

iii) and positivity

$$|A| = D(A,A) \geq 0. \tag{16}$$

There are two simple examples which can be derived from a classical probability measure p. The first is given by the classical (non-interfering) interference function

$$D(A,B) = p(A \cap B)\ . \tag{17}$$

The second example has no immediate interpretation and is given by

$$D(A,B) = p^*(A)\, p(B). \tag{18}$$

Both these decoherence functionals satisfy *i)*, *ii)* and *iii)* above. (Obviously, the classical probability measure is real, and thus there was no need to include a complex conjugation in the second example. However, if we do so, then the expression remains valid in the more general case where p is an arbitrary, additive *complex* function of its argument.)

In this article we will focus on the decoherence functional D and on paths whose positions are restricted to a discrete lattice in both space and time. We will seek the most general translationally invariant processes with nearest neighbor transition amplitudes that form level two generalized measures, i.e. that yield a D satisfying *i)*, *ii)* and *iii)* above. The choice of nearest neighbor transition amplitudes is made for simplicity. The construction presented here could easily be generalised to processes with transitions to any finite number of neighbors.

Our quantal processes are analogues of random walks in classical probability theory. The additional complications we encounter in comparison with the classical case are due mainly to two differences: the more involved nature of the positivity condition, and the possibility that the two walkers corresponding to the two arguments of D can "interact". This "interaction" generalizes the delta function endpoint interaction which characterizes the standard quantum case with its unitary evolution. The new processes go beyond quantum mechanics in that the evolution is not unitary but satisfies a weaker requirement expressing the positivity of the quantal measure.[6] One might think that dropping unitarity allows significant extra freedom, nevertheless, we find the requirements of a well defined level two measure to be remarkably restrictive.

The processes we find are quantal in the sense that they involve transition amplitudes with only pairwise interference. They are also nearest neighbor in that the walker can take at most one step to the left or right, and we are optimistic that an appropriate limit of them will be unitary. Because of their simplicity and closeness to quantum processes of the more traditional sort, we expect that they will yield additional insights into quantum mechanics itself. We hope as well that ideas in this work will help lead us to a physically suitable quantum dynamics for causal sets.

In the next section, we consider further the properties that the transition amplitudes must possess in order to yield a well defined quantal measure, and we introduce to this end a strengthened form of the positivity condition, a condition we call "strong positivity". We also introduce the transfer matrix that defines the Markovian processes we are interested in. In section 3 we find the most general translationally invariant and positive transfer matrix corresponding to a random walk with nearest neighbor transitions. In section 4 we parameterize the general solution to the problem before concluding in section 5.

2 The decoherence functional and strong positivity

First a few definitions. The "completed history" of the walker's motion for $0 \leq t < \infty$ will be called a *trajectory* or *path*. We will assume that the path is *originary*, i.e. begins at the origin, and at each step either stays put or moves one unit to the right or left. A trajectory is thus an infinite sequence of integers, $(0, n_1, n_2, n_3, \cdots)$. It can also be resolved into a sequence of *steps*, $\xi_0 = (0, n_1)$, $\xi_1 = (n_1, n_2)$, $\xi_2 = (n_2, n_3)$, etc. The set of all trajectories will be denoted Ω_∞, and the decoherence functional will therefore have its domain in the set of all sets of trajectories 2^{Ω_∞}. We will also need the notion of truncated trajectory or path, that is a trajectory defined only from the initial time $t = 0$ to some finite "truncation time" T. The set of all such truncated paths will be denoted by Ω_T. Clearly the truncated paths do not live in the same space as the trajectories on which the decoherence functional itself is defined. However, the set of truncated paths Ω_T can be embedded into 2^{Ω_∞} through the notion of *cylinder set*.

[6] This requirement (which we call strong positivity) is a strengthening of condition *iii* above, and is defined in Section 2 below. Besides being strongly positive, the processes we will construct will also satisfy a requirement that is the direct analog of the Markov condition of classical probability theory. Interestingly, unitary processes are normally not Markovian in this sense, a subtlety we discuss further in Section 3.0 below.

The cylinder set $Z(\gamma)$ associated with a truncated path γ of length T is the set of all trajectories which coincide with γ until time T. It should be clear that this mapping Z from truncated paths $\bigsqcup_T \Omega_T$ to sets of trajectories 2^{Ω_∞} is injective and therefore defines a bijection between the space of all truncated paths and that of all cylinder sets, denoted $\mathcal{Z}$. By dint of this equivalence, truncated paths and cylinder sets will normally be identified in the following, and reference to the mapping Z will almost always be omitted. We also make the convention that the empty set is a cylinder set.

Since we are interested in random walks without memory ("Markov processes"), the decoherence functional D can be defined in stages, in a manner we describe in detail in the next subsection 2.1. In analogy with what is done for a classical Markov process, we will first define the decoherence functional inductively on the cylinder sets and then extend it by additivity to more general sets of paths.

Key to this extension are two "algebraic" properties of the cylinder sets: first that the intersection $A \cap B$ of any two cylinder sets is a cylinder set (in fact A and B are either disjoint or nested); and second that the complement of any cylinder set is a finite disjoint union of cylinder sets.[7] It is not difficult to verify these properties if one thinks of the cylinder sets as truncated paths. Notice in particular that a cylinder set of length T is the disjoint union of all the cylinder sets of length $T+1$ that it contains:

$$\gamma^T = \bigsqcup_\sigma \gamma^T \# \sigma, \tag{19}$$

where σ represents all the possible steps the path γ^T of length T can take in passing from T to $T+1$, and the sign # represents the addition of an extra step to a truncated path. (By assumption, there can be only a finite number of possibilities for σ.) Now let $\mathcal{R}$ be the family of all disjoint unions of a finite number of cylinder sets, *i.e.* all subsets $A \subseteq \Omega_\infty$ of the form $A = \sqcup_{i=1}^n \gamma_i$, where the γ_i are cylinder sets. Using the two properties enumerated above, one can prove without difficulty that $\mathcal{R}$ is a "set algebra": it is closed under the operations of union, intersection and complementation. Once D has been defined consistently on cylinder sets, it extends uniquely to $\mathcal{R}$ via bi-additivity (14), and this extension is consistent by the same two properties. (Clearly hermiticity (15) will be preserved by the extension.) Thus D is naturally defined on $\mathcal{R}$.

Notice that D cannot be defined arbitrarily on cylinder sets because one such set can be the disjoint union of a finite number of others, as in (19), and then (14) entails a consistency condition. In our case, we will first define $D(\gamma_1, \gamma_2)$ for γ_1 and γ_2 of equal length, and consistency will then reduce to a simple condition corresponding to (19) that we will make explicit below. The general expression for D on the domain $\mathcal{R}$ will then be

$$D\left(H = \bigsqcup_{i=1}^{n} \gamma_i, K = \bigsqcup_{j=1}^{n'} \gamma'_j\right) = \sum_{ij} D(\gamma_i, \gamma'_j) \ , \tag{20}$$

where the γ's are cylinder sets which, by (19) and (14), can all be taken to have the same length.

In our definition of D on cylinder sets, the hermiticity property (15) will hold by construction. Its general validity will then follow immediately from (20). We thus satisfy by construction

[7] A system of sets with these properties is sometimes called a "semiring" of sets or an "abstract interval family".

both bi-additivity and hermiticity. The positivity condition (16) is a different story, however, and its implementation will occupy us throughout this paper.

The positivity condition we will implement will be somewhat stronger than (16), at least in appearance, and will be called *strong positivity.* Although possibly more restrictive, this condition has proved easier to work with than (16), and we prefer it for that reason. In addition, it has an independent significance as a condition whose satisfaction allows one to derive a Hilbert space from the quantal measure/decoherence functional. And this in turn might be helpful in attempting to extend D and μ to a larger domain of definition than just $\mathcal{R}$. Let us briefly consider these interconnections.

On one hand, many questions of physical importance correspond, not to sets in $\mathcal{R}$ but to "limits" of such sets. For example, the set of all trajectories $\gamma \in \Omega_\infty$ that eventually return to the origin is not a finite but a *countable* union of cylinder sets. Ideally, therefore, one would like to extend D "by continuity" from $\mathcal{R}$ to the full σ-algebra generated by the cylinder sets. On the other hand, the techniques which accomplish this in the case of a classical measure do not go through in the quantum case, because $D(A, B)$ is neither positive nor bounded. A different technique of "completion" is therefore called for. In attempting to meet this need, one might be able to take advantage of the possibility that $\mathcal{R}$ can be made into a Hilbert space with the aid of the decoherence functional D.

The construction of the Hilbert space $\mathcal{H}$ proceeds in "GNS" (Gel'fand-Naimark-Segal) fashion. One interprets D as an "inner product on $\mathcal{R}$" and obtains $\mathcal{H}$ as the set of formal linear combinations of elements of $\mathcal{R}$. More exactly, one quotients this space by the subspace of null vectors and then completes the quotient to arrive at $\mathcal{H}$. If one does this in the unitary case, the resulting Hilbert space $\mathcal{H}$ is none other than the one normally employed as the state-space of the quantum system in question. Thus, one recovers the quantum Hilbert space $\mathcal{H}$ directly from the decoherence functional D, without any reference to canonical commutation relations, classical phase spaces, or other auxiliary structures [8]. Now, nothing limits this construction to the unitary case, but in order for it to succeed in general, (16) must be strengthened to the requirement that we will call strong positivity (and which is automatically satisfied in the unitary case). As already mentioned, we will see that this requirement also emerges naturally in the attempt to guarantee (16) for our quantal random walk.

Definition 1 *A decoherence functional D is* **strongly positive** *if it fulfills either (and therefore both) of the following two equivalent conditions:*

i) for any finite collection of sets $A_i \in \mathcal{R}$, $1 \leq i \leq n$, the (hermitian) matrix $N_{ij} = D(A_i, A_j)$ is positive;

ii) the (finite hermitian) matrix $M_{\gamma_1,\gamma_2} = D(\gamma_1, \gamma_2)$, $\gamma_i \in \Omega_T$ is a positive matrix for all T.

Note that, as the names suggest, strong positivity implies weak positivity, as can be seen by simply taking $n = 1$ in the first definition of strong positivity. It should also be clear that the first definition of strong positivity implies the second by choosing the finite sets A_i to be the cylinder sets γ_i in Ω_T. It remains only to prove the reverse implication.

Let us therefore suppose that the matrix M_{γ_1,γ_2} is positive and let $N_{ij} = D(A_i, A_j)$. Writing the A_i as sets of truncated trajectories γ^T for T sufficiently large, and introducing a generic

[8] Compare the analogous construction of [17].

column vector ψ with components ψ_i, we have

$$\psi^\dagger N\psi = \sum_{\gamma_1,\gamma_2\in\Omega_T} M_{\gamma_1,\gamma_2}\left(\sum_{i,\gamma\in A_i}\psi_i\delta_{\gamma_1,\gamma}\right)^*\left(\sum_{j,\gamma'\in A_j}\psi_j\delta_{\gamma_2,\gamma'}\right) \tag{21}$$

$$= \sum_{\gamma_1,\gamma_2\in\Omega_T} M_{\gamma_1,\gamma_2}\rho^*(\gamma_1)\rho(\gamma_2) \geq 0, \tag{22}$$

where the positivity of M was used and we defined

$$\rho(\gamma') = \sum_{i,\gamma\in A_i}\psi_i\delta_{\gamma',\gamma}\ . \tag{23}$$

This concludes the demonstration of the equivalence between the two definitions.

As already noted, we have the following obvious theorem:

Theorem 1 *A strongly positive decoherence functional is positive.*

Indeed, for any set of truncated paths and $A = \sqcup\gamma_i$,

$$\mu(A) = \sum_{ij} D(\gamma_i,\gamma_j) = v^*_{\gamma_1} M_{\gamma_1\gamma_2} v_{\gamma_2} \geq 0, \tag{24}$$

where the notation is that of the second definition *ii)* and v_γ is a vector made of 0s and 1s which is 1 if $\gamma \in A$ and 0 otherwise. Thus, in contrast with strong positivity, we see that plain positivity only requires that the quadratic form associated with the hermitian matrix $M_{\gamma_1\gamma_2}$ be positive when applied to column vectors made of 0s and 1s. Of course, an even simpler proof is possible, if we start from the first form of Definition 1: simply apply it to the single set A and observe that the 1×1 positive matrix N is simply $[\mu(A)]$.

Since strong positivity is associated with a Hilbert space structure, some familiar properties arise from it, such as the following.

Theorem 2 *For any two sets A and B in $\mathcal{R}$, $|D(A,B)|^2 \leq |A|\,|B|$.*

This is just the statement that the determinant of the positive hermitian 2×2 matrix obtained from definition *i)* of strong positivity and the collection of sets (A, B) is positive. As observed in footnote 5, this theorem guarantees us a quantum measure theory in the sense of [5].

2.1 Decoherence functional from a transfer matrix

In the following, we will be interested in a process whose decoherence functional on truncated paths is defined iteratively through a transfer matrix, which will be denoted a. Since this is in close analogy to the Markov property of classical probability theory, one may call such a process "Markovian".

Before proceeding, it is convenient to expand on our notation. A generic truncated trajectory will be written as γ. If it has length T, this will be indicated by a superscript γ^T. The position of a path γ at a given time t will be written as $\gamma(t)$. Since we are interested in a quantum random walk with nearest neighbor transitions, at each step, a truncated trajectory will only be allowed three possible moves: to the same position, or to the nearest left or right one. Its successive moves can thus be expressed by a finite time sequence of integers $\sigma(t) \in \{-1, 0, +1\}$. Since we restrict our consideration to originary paths, i.e. paths γ beginning at the origin, a truncated trajectory is entirely defined by its associated sequence $\sigma_\gamma(t)$,

$$\begin{aligned} \gamma(t+1) &= \gamma(t) + \sigma_\gamma(t) \qquad (25) \\ \gamma(t) &= \sum_{t=0}^{t-1} \sigma_\gamma(t). \qquad (26) \end{aligned}$$

As represented already in (19), a truncated path of length T can be extended to a truncated path of length $T+1$ by defining its position at the next step $T+1$, which as explained above is just given by an integer $\sigma \in \{-1, 0, +1\}$. The sequence of length $T+1$ which coincides with γ^T for the first T steps and which has position $\gamma^T(T) + \sigma$ at time $T+1$ will be denoted $\gamma^T\#\sigma$. With these choices and definitions, Eq. (19) becomes simply

$$\gamma^T = (\gamma^T\# - 1) \sqcup (\gamma^T\#0) \sqcup (\gamma^T\#1)\ . \qquad (27)$$

Conversely, a truncated path γ^T of length T can be truncated further to a length $T-1$ path γ^{T-1}, by taking the latter to coincide with γ^T on the first $T-1$ steps.

Now, a transfer matrix will give transition amplitudes from time T to time $T+1$, for the *pair* of truncated paths (γ_1, γ_2). Since we are considering a one step Markov process, this amplitude should only depend on the positions of the truncated paths at times T and $T+1$. Furthermore, assuming spatio-temporal homogeneity, it should not depend explicitly on the step T considered, and it should depend only on the relative position of the two paths, not on their absolute location. Thus the transfer matrix can be written as $a(n_1, \sigma_1, n_2, \sigma_2)$ where n_i are integers and a only depends on n_i through the difference $n_1 - n_2$:

$$a(n_1, \sigma_1, n_2, \sigma_2) = a(n_2 - n_1, \sigma_1, \sigma_2)\ . \qquad (28)$$

In the rest of the paper, we will use for a whichever notation is most convenient at the time.

With these notations, the decoherence functional on cylinder sets is given recursively by

$$D(\gamma_1^T\#\sigma_1, \gamma_2^T\#\sigma_2) = D(\gamma_1^T, \gamma_2^T) a(\gamma_1^T(T), \sigma_1, \gamma_2^T(T), \sigma_2)\ . \qquad (29)$$

The hermiticity condition (15) then requires that

$$a(n_2, \sigma_2, n_1, \sigma_1) = a^*(n_1, \sigma_1, n_2, \sigma_2)\ . \qquad (30)$$

As for the self-consistency condition (19), it constrains the transfer matrix to satisfy the equation,

$$D(\gamma_1^T, \gamma_2^T) \left(\sum_{\sigma_1, \sigma_2} a(\gamma_1^T(T), \sigma_1, \gamma_2^T(T), \sigma_2) - 1 \right) = 0 \qquad (31)$$

for any time T and any pair of truncated paths (γ_1^T, γ_2^T) and integers (σ_1, σ_2). In general, there will always be at least one time T and pair of truncated paths (γ_1^T, γ_2^T) ending at a given pair of lattice positions (n_1, n_2) such that $D(\gamma_1^T, \gamma_2^T) \neq 0$; and therefore our constraint will simplify to

$$\sum_{\sigma_1, \sigma_2} a(n_1, \sigma_1, n_2, \sigma_2) = 1\ . \qquad (32)$$

However, this is not always true, and there exist important special cases in which it fails. One such is the classical random walk, for which there is no interference and D assumes the degenerate form (17). In this case (since distinct members of Ω_T are disjoint as cylinder sets), $D(\gamma_1^T, \gamma_2^T)$ vanishes unless $\gamma_1^T = \gamma_2^T$, and the transfer matrix is necessarily diagonal in (σ_1, σ_2). The constraint (31) then reduces to

$$\sum_{\sigma} a(n, \sigma, n, \sigma) = 1 \; . \tag{33}$$

In fact, if we write the transfer matrix in the form $a(n_2 - n_1, \sigma_1, \sigma_2)$, we see that it does not depend on n at all in this case, and (33) reduces further to $\sum_{\sigma} a(\sigma) = 1$, which is just the Markov sum rule for a classical stochastic process. Notice that, here, the transfer matrix is strictly speaking undefined unless $n_1 = n_2$.

As we have just seen, the classical random walk is characterized by the condition that the "walker" and "antiwalker" never separate. Between this and the generic case, there may exist intermediate cases in which the walker and antiwalker can move apart, but never by more than some fixed distance d. Such processes, if they exist, might offer an interesting transition between the fully classical and fully quantum situations.

Obviously, the transfer matrix a carries full information about the decoherence functional D, and it would be useful to translate the strong positivity condition on D to a condition on a. By doing so, one obtains theorem 3 below. In the statement of this theorem, a is to be regarded as a matrix with rows and columns labeled by the pairs $\xi_1 = (n_1, \sigma_1)$ and $\xi_2 = (n_2, \sigma_2)$ respectively. That is, the rows and columns correspond to *steps* of the two respective paths γ_1 and γ_2, not, as one might think, to their successive *locations*, which would label the rows and columns by successive values of the pair (n_1, n_2). Notice that a is an infinite matrix. We will define such a matrix to be *positive* if every finite principal submatrix is positive as a finite matrix. Equivalently, $\sum_{\xi\eta} a_{\xi\eta} \psi_\xi^* \psi_\eta \geq 0$ for every "column vector" ψ having only a finite number of nonzero components ψ_ξ.

Notice also that the positivity condition on D which figures in Theorem 3 is not "weak" positivity (16) but strong positivity as defined in the previous subsection. We do not know whether there exists any simple translation of weak positivity into a property of the transfer matrix, and this is one reason why we have been led to work with strong positivity instead.

Theorem 3 *If the transfer matrix a is positive, then the corresponding decoherence functional D defined through (29) is strongly positive.*

In order to prove this theorem we will build up the decoherence functional as a kind of product involving the transfer matrix. However, the product in question is not the ordinary matrix product, but rather what is called the Hadamard product, denoted $\sharp$ in the following, which multiplies two matrices $M_{ij}^{(1)}$ and $M_{ij}^{(2)}$ entry by entry:

$$(M^{(1)} \sharp M^{(2)})_{ij} = M_{ij}^{(1)} M_{ij}^{(2)} . \tag{34}$$

The proof of the theorem then hinges on the following lemma.

Lemma 1 *The Hadamard product of two positive matrices is also a positive matrix.*

The proof is quite simple. Since $M^{(1)}$ is positive and therefore hermitian, it can be put into the following diagonal form[9]

$$M^{(1)} = \sum_i \lambda_i v^{(i)} v^{(i)\dagger}, \tag{35}$$

where the $\lambda_i \geq 0$ are its eigenvalues and the $v^{(i)}$ are a corresponding basis of orthonormal eigenvectors. Then, given a generic vector ψ,

$$\psi^\dagger (M^{(1)} \sharp M^{(2)}) \psi = \sum_{ijk} \lambda_i (\psi_j v_j^{(i)})^* M_{jk}^{(2)} (\psi_k v_k^{(i)}) \tag{36}$$

$$= \sum_i \lambda_i \rho^{(i)\dagger} M^{(2)} \rho^{(i)} \geq 0, \tag{37}$$

since each of the terms in the sum is positive by definition of the positivity of $M^{(2)}$, and where

$$\rho^{(i)} = \psi \sharp v^{(i)}. \tag{38}$$

Proof of the Theorem: The theorem is proved by checking that if a is positive then the matrices $D(\gamma_1, \gamma_2)$ for $\gamma_i \in \Omega_T$ are positive for all T. This, in turn, is proved by induction on T. For $T = 0$, the result is trivial since then Ω_T contains only one element, with measure one (as conventionally normalized).

Let us now suppose that the theorem is true at step T: D is positive on Ω_T. Then we need to prove that the matrix

$$D(\gamma_1^{T+1}, \gamma_2^{T+1}) = D(\gamma_1^T, \gamma_2^T) a(\gamma_1(T), \sigma_1(T), \gamma_2(T), \sigma_2(T)) \tag{39}$$

is a positive matrix. To use the Hadamard positivity lemma on the right hand side, both matrices a and D must be extended to matrices of the size of Ω_{T+1}, which we will call a^e and D^e. This is easily done by some appropriate truncations:

$$a^e(\gamma_1^{T+1}, \gamma_2^{T+1}) = a(\gamma_1^{T+1}(T), \gamma_1^{T+1}(T+1) - \gamma_1^{T+1}(T), \gamma_2^{T+1}(T), \gamma_2^{T+1}(T+1) - \gamma_2^{T+1}(T)) \tag{40}$$

$$D^e(\gamma_1^{T+1}, \gamma_2^{T+1}) = D(\gamma_1^T, \gamma_2^T). \tag{41}$$

Then, by the Lemma, it suffices to prove that the two matrices a^e and D^e are positive.

This is actually a simple matter since for any vector ψ indexed on Ω_{T+1},

$$\psi^\dagger a^e \psi = \sum_{\gamma_i \in \Omega_{T+1}} \psi_{\gamma_1}^* a(\gamma_1(T), \sigma_1(T), \gamma_2(T), \sigma_2(T)) \psi_{\gamma_2} \tag{42}$$

$$= \sum_{n_i, \sigma_i} a(n_1, \sigma_1, n_2, \sigma_2) \left(\sum_{\gamma \in \Omega_{T-1}} \psi_{\gamma \# n_1 \# (n_1 + \sigma_1)} \right)^* \left(\sum_{\gamma' \in \Omega_{T-1}} \psi_{\gamma' \# n_2 \# (n_2 + \sigma_2)} \right) \tag{43}$$

$$= \sum_{n_i, \sigma_i} a(n_1, \sigma_1, n_2, \sigma_2) \rho_{n_1, \sigma_1}^* \rho_{n_2, \sigma_2} \geq 0 \,. \tag{44}$$

Here we have used a slightly different version of the # notation introduced after equation (19), according to which $\gamma^{T+1} = \gamma^{T-1} \# \gamma^{T+1}(T) \# (\gamma^{T+1}(T) + \sigma(T))$. In the final step of the proof, the inequality followed from the positivity of a as applied to the vector

$$\rho_{n,\sigma} = \sum_{\gamma \in \Omega_{T-1}} \psi_{\gamma \# n \# (n+\sigma)} \,. \tag{45}$$

[9]Because the matrices here are playing the role of quadratic forms, the λ's have no real significance, and could be absorbed into the v's

The positivity of D^e is proved in a similar way, but performing the sums on $\sigma_i(T)$ first.

This concludes the induction and the proof. Notice that the sum-rule (31) played no role in the proof and a need not have satisfied it. Notice also that the restriction to a nearest neighbor transfer matrix could have been lifted with little difficulty.

We believe that the converse of the Theorem 3 is likely to hold as well, at least generically; however we do not have a clean proof of this. If we are right, then, in seeking a transfer matrix a that will yield a strongly positive decoherence functional D, we lose no generality in assuming that a itself is a positive matrix.

In any case, we have established that to obtain a bi-additive, hermitian symmetric, positive decoherence functional from a transfer matrix, it suffices to find a positive transfer matrix satisfying (31) or (32). Let us now concentrate on doing so.

3 The transfer matrix and its Fourier transform

In the Introduction, we raised the question whether the quantal process corresponding to the Schrödinger equation could arise as the continuum limit of a quantal random walk. Because of the delta function at the truncation time T in the Schrödinger decoherence functional (cf. equation (12)), one might try to write down a transfer matrix incorporating an analogous δ-function (or rather Kronecker δ), but this would not accomplish anything, because such a δ-function would immediately throw us back to the classical case (17).

This highlights a subtle difference between the type of process we are considering in this paper and the type of process considered in ordinary unitary quantum mechanics (with or without added decoherence). In our scheme, the central object is the decoherence functional D (or the corresponding quantal measure μ), and our transfer matrix a evolves D directly from one instant of time to the next. The fact that D can be built up step by step in this manner is what we refer to in terming our quantal processes "Markovian".[10] A particular consequence is that one could define a "density matrix" $\rho(n_1, n_2, t)$ which would evolve from one time to the next via the action of transfer matrix a and which would record the value of D on classes of paths ending at n_1 and n_2, respectively.

Calling such a ρ a density matrix could be misleading, however, since it does not correspond to what is normally called "density matrix" in the context of unitary quantum mechanics. Indeed, unitary evolution (unlike the classical random walk) is *not* contained within our general transfer matrix scheme as a special case; and no special case of our quantal random walk could be unitary, *even if* we dropped the bound on the step size.[11] The reason is that the density matrix in the normal sense (call it $\rho'(n_1, n_2)$) does not vanish when $n_1 \neq n_2$, whereas the decoherence functional of unitary quantum mechanics does, because of the final δ-function that occurs in (12).

[10] From the standpoint of the quantal measure μ, our scheme falls short of being fully Markovian, since it is the decoherence functional D which evolves locally in time, and this evolution makes essential reference to extra information (the imaginary part of D) not contained in the measure itself. (Of course, because of interference, even μ contains extra information not present in the measures of the individual trajectories, and this furnishes a quite different reason why one might view quantal processes as not Markovian in an important physical sense, cf. the discussion of "fuzzing" in [13].)

[11] The same applies to extensions of unitary quantum mechanics which incoporate "environmental dechoherence"

Indeed, the normal density matrix ρ' is related only indirectly to the decoherence functional of unitary quantum mechanics and has no meaning in itself, within a "histories" formulation. Rather it is a kind of phantom, telling us what the decoherence functional "would be" if one were not going to impose the final delta-function at some future time T. But of course, one does need to impose this condition in the future (in the unitary context), and because of it, unitary evolution could be seen as not truly Markovian. For the same reason, unitary evolution could also be seen as unnatural, in agreement with the observation that the final δ-function that couples γ_1 to γ_2 is a rather violent and discontinuous interaction, compared to what one might have expected for such a coupling.

By these comments, we do not mean to imply that unitary behavior cannot arise from our type of process, but only that it cannot be obtained by specialization. (It could be at best some sort of singular limit, since the transfer matrix, as we have employed that term, would be either infinite, zero, or undefined if one tried to define it for the case of unitary evolution.) Rather, we would expect it to emerge only after some suitable coarse-graining in both space and time. This would yield an effective decoherence functional on coarse-grained trajectories, which would be effectively unitary if it took the form (12), in other words if the interaction between "walker" and "antiwalker" reduced to a final delta-function. (Equivalently stated: the amplitude should factor *except for* the final delta-function.)

But how could one design a transfer matrix that would lead to such a result? Could one begin with "non-interacting" paths γ_1 and γ_2, each of which evolved approximately according to the Schrödinger equation, and then adjoin a suitably "attractive" interaction that at late times would condense into a smeared delta-function? The following developments are motivated by this prospect. First, we consider "free Schrödinger evolution" and then ask how to perturb it while preserving positivity. In the end however, it proved easier to find the most general positive transitive transfer matrix directly, and we present this in Section 3.2.

3.1 Transition amplitudes for the Schrödinger process

We are interested in finding a quantum random walk which could describe, in the continuum limit, a particle satisfying the Schrödinger equation,

$$\frac{\partial\psi}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2\psi}{\partial x^2}. \tag{46}$$

To this end, let us begin by approximating the Schrödinger equation via the method of finite differences, using the lattice, $(m\Delta t, n\Delta x)$, $m \in \mathbb{N}$, $n \in \mathbb{Z}$. We have, at leading order,

$$\frac{\partial\psi(t,x)}{\partial t} = \frac{\psi(t+\Delta t,x)-\psi(t,x)}{\Delta t} \tag{47}$$

$$\frac{\partial^2\psi(t,x)}{\partial x^2} = \frac{\psi(t,x+\Delta x)+\psi(t,x-\Delta x)-2\psi(t,x)}{(\Delta x)^2}\ , \tag{48}$$

which yields to leading order

$$\psi(t+\Delta t,x) = (1-2ip)\psi(t,x)+ip(\psi(t,x+\Delta x)+\psi(t,x-\Delta x)) \tag{49}$$

$$\text{with } p = \frac{\hbar\Delta t}{2m(\Delta x)^2}. \tag{50}$$

From this expression, a set of one-particle transition amplitudes can be extracted as

$$p(\pm 1) = ip \tag{51}$$

$$p(0) = 1 - 2ip. \tag{52}$$

These transition amplitudes sum to one like classical transition probabilities, but of course they are neither real nor positive.

Let us denote by $p(\gamma)$ the amplitude of a truncated path obtained from the Schrödinger amplitudes $p(\pm 1, 0)$. The quantum decoherence functional we are ultimately aiming for is something like

$$D(\gamma_1^T, \gamma_2^T) = p^*(\gamma_1^T)p(\gamma_2^T)\delta_{\gamma_1^T(T),\gamma_2^T(T)} \ , \tag{53}$$

where δ is the Kronecker symbol. However, as we know, this decoherence functional with its delta-function interaction depending only on the end-points of the truncated paths is not viable for a nearest neighbor random walk, since it necessarily comes into conflict with the additivity condition (14), which in this case is equivalent to unitarity. (Nor, as we have already observed, would it be appropriate for a process which could be called Markovian in our sense of the word.) However (cf. (18)), there is another decoherence functional which can be derived from the transition amplitudes $p(\gamma)$, given simply by

$$D(\gamma_1^T, \gamma_2^T) = p^*(\gamma_1^T)p(\gamma_2^T) \ . \tag{54}$$

It would not reproduce the Schrödinger process in the continuum limit, but it is Markovian, corresponding to the transfer matrix

$$a^{(0)}(n_1, \sigma_1, n_2, \sigma_2) = p^*(\sigma_1)p(\sigma_2) \ , \tag{55}$$

which, so far, does not depend on the particle positions $n_{1,2}$. Notice three things: first that the sum-rule (32) is automatically satisfied by (55) and doesn't need to be imposed separately; second that $a^{(0)}$ is positive, as expected from the fact that the decoherence functional (54) from which it derives is itself obviously strongly positive; and third that the symmetry $p(+1) = p(-1)$ expresses a no–drift condition on our quantal walk.

This transfer matrix does not describe the quantum process we are interested in. However, if it is perturbed in such a way as to become attractive, then at late times, the decoherence functional should vanish when the two "particles" are far from one another, and this is exactly the type of decoherence functional (53) we are seeking. Perturbing the transfer matrix while keeping it positive, however, is far less trivial than it might seem, and this is the question we now turn to.

3.2 Positivity of the transfer matrix

Henceforth, we will assume that the transfer matrix is defined for all n and σ, this being the generic case. This implies in particular that the consistency condition (32) will have to hold for all values of its arguments.

We saw in Eq. (28) that the transfer matrix depends on the two particle-positions only through the difference $n_2 - n_1$. Using the reduced notation for the transfer matrix, we can introduce the Fourier transform (of period 2π),

$$a(\theta, \sigma_1, \sigma_2) = \sum_{n=-\infty}^{+\infty} a(n, \sigma_1, \sigma_2)\mathrm{e}^{in\theta} \tag{56}$$

and its inverse,

$$a(n,\sigma_1,\sigma_2)=\frac{1}{2\pi}\int_0^{2\pi}a(\theta,\sigma_1,\sigma_2)\mathrm{e}^{-in\theta}d\theta. \tag{57}$$

Under Fourier transform, the hermiticity condition Eq. (30) becomes the requirement that the 3×3 matrix $a(\theta,\sigma_1,\sigma_2)$ be hermitian for all θ. The sum rule, equation (32), can also be Fourier transformed without difficulty, yielding:

$$\sum_{-1\le\sigma_1,\sigma_2\le 1}a(\theta,\sigma_1,\sigma_2)=2\pi\delta(\theta), \tag{58}$$

where δ is the usual delta distribution of Dirac. Observe that this equation just fixes the value of the quadratic form associated with the hermitian matrix $a(\theta)$ on the vector $(1,1,1)$.

Now consider the requirement that a be a positive matrix. Introducing a generic vector $\psi_{n,\sigma}$ and its associated Fourier series

$$\psi(\theta,\sigma)=\sum_{n=-\infty}^{+\infty}\psi_{n,\sigma}\mathrm{e}^{in\theta}\ , \tag{59}$$

we obtain this condition in the form:

$$\psi^\dagger a\psi = \frac{1}{2\pi}\int_0^{2\pi}d\theta\sum_{n_i,\sigma_i}a(\theta,\sigma_1,\sigma_2)\psi^*_{n_1,\sigma_1}\psi_{n_2,\sigma_2}\mathrm{e}^{-i(n_2-n_1)\theta} \tag{60}$$

$$= \frac{1}{2\pi}\int_0^{2\pi}d\theta\sum_{\sigma_i=-1}^{1}\psi^*_{\sigma_1}(\theta)\psi_{\sigma_2}(\theta)a(\theta,\sigma_1,\sigma_2)\ge 0\ . \tag{61}$$

This is certainly satisfied for any ψ if the hermitian 3×3 matrix $a(\theta,\sigma_1,\sigma_2)$ is positive for all θ. Conversely, if that matrix fails to be positive semi-definite at any θ_0, then there exists ρ_i a three component vector such that $\rho_i^\dagger a(\theta_0,i,j)\rho_j<0$. Then the vector

$$\psi_{n,\sigma}=\frac{\rho_\sigma}{2\pi}\mathrm{e}^{-in\theta_0} \tag{62}$$

to which corresponds the Fourier transform $\psi(\theta,\sigma)=\rho_\sigma\delta(\theta-\theta_0)$, will certainly yield $\psi^\dagger a\psi<0$, proving that a is not positive. Thus, we have demonstrated the following

Theorem 4 *If the Fourier transform, $a(\theta,\sigma_1,\sigma_2)$, of the interaction matrix $a(n,\sigma_1,\sigma_2)$ is a positive 3×3 hermitian matrix, for all values of θ, then the corresponding transfer matrix is also positive, and conversely.*

Actually, our demonstration was not rigorous, mainly because $a(\theta)$ need not (and indeed cannot) be continuous. Nonetheless, it seems clear that the theorem does hold rigorously if $a(\theta)$ is interpreted as a matrix-valued measure, because it is then nothing more than the matrix generalization of the following classical result.[12]

[12] The condition in the Herglotz theorem that f be "of positive type" means that $M(n_1,n_2):=f(n_1-n_2)$ be a positive matrix. In other words, it is precisely the condition we need for positivity of the transfer matrix. We have quoted the Herglotz theorem from [18].

Theorem 5 *(***Herglotz***) A function f on the integers $\mathbb{Z}$ is of positive type iff it is the Fourier transform of a finite (positive) measure on the circle S^1, i.e. f is of positive type iff it has the form*

$$f(n) = \int_{-\pi}^{\pi} d\alpha(\theta) \exp(in\theta)$$

where α is a bounded monotone increasing function on $[-\pi, \pi]$.

The form $d\alpha(\theta)$ allows $a(\theta)$ to contain delta-functions, but nothing more singular. To see why this should be so, consider a transfer matrix of the following form:

$$a(\theta, i, j) = a_c(\theta, i, j) + \sum_{k=0}^{l} M_{ij}^{(k)} \delta^{(k)}(\theta - \theta_0), \tag{63}$$

where $a_c(\theta, i, j)$ is a positive continuous (or even piecewise continuous) contribution, θ_0 is a fixed number, $\delta^{(k)}$ is the k-th derivative of the Dirac distribution and l is a given integer, for which $M_{ij}^{(l)} \neq 0$. Let us prove then that the positivity condition implies that $l = 0$, i.e. that nothing more singular than a δ-function can be present, and that $M_{ij}^{(0)}$ must be a positive hermitian matrix.

To that end, let us suppose that $l > 0$ and introduce smooth test functions $\psi_l^{\pm}(\theta)$ with a support on the interval $[-1, 1]$ and such that

$$\left.\frac{d^k \psi_l^{\pm}}{d\theta^k}\right|_0 = \delta_{0,k} \pm \delta_{l,k}, \;\; 0 \leq k \leq l \tag{64}$$

where δ is the Kronecker symbol. Then taking $\psi_\sigma(\theta) = \rho_\sigma \psi_l^{\pm}(\alpha(\theta - \theta_0))$ with $\alpha > 0$ a real parameter, the inequality (61) yields

$$\psi^\dagger a \psi = \frac{1}{2\pi} \rho_i^\dagger \rho_j (\int_0^{2\pi} d\theta |\psi_l^{\pm}(\alpha(\theta - \theta_0))|^2 a_c(\theta, i, j) + M_{ij}^{(0)} \pm 2\alpha^l M_{ij}^{(l)}) \geq 0. \tag{65}$$

Bounding from above the first term on the left–hand side then yields

$$\rho_i^\dagger \rho_j (\min(\frac{2}{\alpha}, 2\pi) \sup_{0 \leq \theta \leq 2\pi} [\, |\psi_l^{\pm}(\alpha(\theta - \theta_0))|^2 a_c(\theta, i, j)] + M_{ij}^{(0)} \pm 2\alpha^l M_{ij}^{(l)}) \geq 0. \tag{66}$$

In the large α limit, the linear term, which dominates the left–hand side, can only be positive if it is identically zero, thus yielding that $\rho_i^\dagger M_{ij}^{(l)} \rho_j = 0$ for any vector ρ, which in turn implies that $M_{ij}^{(l)} = 0$ in contradiction with its definition. Thus $l = 0$. Furthermore, with $l = 0$, the inequality (66) becomes

$$\rho_i^\dagger \rho_j (\min(\frac{2}{\alpha}, 2\pi) \sup_{0 \leq \theta \leq 2\pi} [\, |\psi_l^{\pm}(\alpha(\theta - \theta_0))|^2 a_c(\theta, i, j)] + M_{ij}^{(0)}) \geq 0, \tag{67}$$

which in the limit $\alpha \to +\infty$ yields immediately that $M_{ij}^{(0)}$ is a positive matrix as desired.

It should also be clear that this proof can be generalized without any difficulty to include a finite number of delta functions at different points, and for convenience, we will not consider anything more general than this. Thus, we have the

Corollary 1 *The Fourier transform of a distribution of the form*

$$a(\theta, i, j) = a_c(\theta, i, j) + \sum_{k=0}^{L} a_{ij}^{(k)} \delta(\theta - \theta_k), \tag{68}$$

where $a_c(\theta, i, j)$ is continuous (or piecewise continuous), hermitian and positive for all θ, and where the $a_{ij}^{(k)}$ are positive hermitian matrices, is a positive transfer matrix.

Strictly speaking, we do not have a transfer matrix until the sum rule (32) is also satisfied. The conditions needed to insure this are implemented explicitly in the next section.

Although the form (68) is not quite exhaustive, it furnishes a large class of positive transfer matrices, and therefore a large class of strongly positive decoherence functionals.

4 Parameterizing the positive transfer matrices

Before turning to the general case, let us briefly treat the classical random walk, which is a special case of our Markovian process, as we have seen. In order to be able to apply the above Corollary without modification, we need the transfer matrix to be defined for all possible arguments, n and σ, and we may choose to accomplish this by setting it to 0 outside its natural domain of definition. It is clear that it will be positive after this extension if and only if it was positive before the extension. When defined in this way, it remains diagonal and independent of n, taking specifically the following form:

$$a(n_1, \sigma_1, n_2, \sigma_2) = p_\sigma \delta_{\sigma\sigma_1} \delta_{\sigma\sigma_2} \ , \tag{69}$$

where δ is the Kronecker symbol. In the absence of any position dependence, the Fourier transform is trivial and yields $a(\theta, \sigma_1, \sigma_2) = 2\pi p_\sigma \delta_{\sigma\sigma_1} \delta_{\sigma\sigma_2} \delta(\theta)$. The corollary then tells us that $p_\sigma \geq 0$, where, to satisfy the sum rule (32), or equivalently in this case (33), we need also $\sum_\sigma p_\sigma = 1$.

Thus we recover exactly the expected form for a classical random walk. For an isotropic walk, the rightward and leftward probabilities must coincide, and the parameters $p(\sigma)$ of the process simplify to just $(p, 1-2p, p)$, with a single degree of freedom $p \in [0, 1/2]$.

Now let us turn to the generic case, whose sum rule is given by equation (32).

4.1 The generic case

At this point, it is convenient to split the Fourier transformed function $a(\theta, \sigma_1, \sigma_2)$ of (68) into a fixed part $a^{(0)}$ chosen as simply as possible to satisfy the Fourier transform of (32), namely

$$\sum_{\sigma_1, \sigma_2} a^{(0)}(\theta, \sigma_1, \sigma_2) = 2\pi\delta(\theta) \ , \tag{70}$$

and a variable part $a_i(\theta, \sigma_1, \sigma_2)$ which satisfies the homogeneous version of the same equation:

$$\sum_{-1 \leq \sigma_1, \sigma_2 \leq 1} a_i(\theta, \sigma_1, \sigma_2) = 0 \ . \tag{71}$$

Thus, we shall write the general solution in the form

$$a(\theta,\sigma_1,\sigma_2) = 2\pi a^{(0)}_{\sigma_1\sigma_2}\delta(\theta) + a_i(\theta,\sigma_1,\sigma_2) \ , \tag{72}$$

where a_i can be split further into a continuous part and a distributional part,

$$a_i(\theta,\sigma_1,\sigma_2) = a_c(\theta,\sigma_1,\sigma_2) + \sum_{k=1}^{L} a^{(k)}_{\sigma_1\sigma_2}\delta(\theta-\theta_k) \ , \tag{73}$$

where the θ_k for $k = 1\cdots L$ are any distinct nonzero angles. We have seen that, in order to generate a proper decoherence functional, all the 3×3 matrices $a^{(j)}$ must be hermitian positive (including for $j = 0$), as must also the matrices $a_c(\theta,\sigma_1,\sigma_2)$ for each θ. Furthermore, these matrices must satisfy the constraint equations

$$\sum_{-1\le\sigma_1,\sigma_2\le 1} a^{(0)}_{\sigma_1,\sigma_2} = 1 \tag{74}$$

$$\sum_{-1\le\sigma_1,\sigma_2\le 1} a_c(\theta,\sigma_1,\sigma_2) = \sum_{-1\le\sigma_1,\sigma_2\le 1} a^{(k)}_{\sigma_1\sigma_2} = 0 \ . \tag{75}$$

Simple choices for the matrix $a^{(0)}$ are easy to find, for instance $a^{(0)}_{ij} = 1/9$. In practice, the choice of $a^{(0)}$ would be adapted to the problem under consideration. For instance, as discussed in section 3, it would be natural to expect the transfer matrix whose coarse-grained evolution reproduces the Schrödinger process to be a perturbation of the transfer matrix given in (55). Thus, one might use the latter for $a^{(0)}$, since it fulfills all the requirements, as observed earlier.

As for the variable part a_i, it must satisfy the homogeneous constraint (71). We can simplify this condition by observing that it merely signifies that the vector $(1,1,1)$ is in the kernel of the positive quadratic form associated with the hermitian matrix $a_i(\theta)$. This in turn implies that $(1,1,1)$ is a minimum of the quadratic form, and therefore an eigenvector of $a_i(\theta)$ for the eigenvalue zero. Conversely, if $(1,1,1)$ is a zero eigenvector of a_i then the latter obviously satisfies the constraint. To summarize, the constraint (71) is equivalent to the three equations

$$\sum_{-1\le\sigma\le 1} a_i(\theta,\tau,\sigma) = 0 \ , \tag{76}$$

or equivalently,

$$\sum_{-1\le\sigma\le 1} a_c(\theta,\tau,\sigma) = \sum_{-1\le\sigma\le 1} a^{(k)}(\tau,\sigma) = 0 \tag{77}$$

for all $\tau\in\{-1,0,1\}$.

It follows that both these matrices must have the form $0_{(1,1,1)} \oplus H_{(1,1,1)^\perp}$, where H is an arbitrary positive hermitian matrix on the two–dimensional space $(1,1,1)^\perp$. Now, the general two–dimensional positive hermitian matrix can be parametrized as

$$\begin{pmatrix} A & \sqrt{3}(R-iI) \\ \sqrt{3}(R+iI) & 3B \end{pmatrix}, \tag{78}$$

where A, B, R, I are real numbers subject to the inequalities

$$A \ge 0,\ \ AB \ge (R^2+I^2) \ . \tag{79}$$

Then, employing $((1/\sqrt{2},0,-1/\sqrt{2}),(1/\sqrt{3},-2/\sqrt{3},1/\sqrt{3}))$ as an orthonormal basis for $(1,1,1)^\perp$, one straightforwardly derives the general solution for the matrices a_c and $a^{(k)}$ as

$$\begin{pmatrix} \frac{A+B}{2}+R & -B-R+iI & \frac{B-A}{2}-iI \\ -B-R-iI & 2B & -B+R+iI \\ \frac{B-A}{2}+iI & -B+R-iI & \frac{A+B}{2}-R \end{pmatrix} , \tag{80}$$

still subject to (79).

In the following, we will further require that the reflection symmetry of the non–interacting model be preserved by the interaction term, i.e. that there be no drift. This implies that the transfer matrix be symmetric under the reflection $n \to -n$:

$$a(-n_1,-\sigma_1,-n_2,-\sigma_2) = a(n_1,\sigma_1,n_2,\sigma_2) \ . \tag{81}$$

Under Fourier transformation, this becomes

$$a(\theta,\sigma_1,\sigma_2) = a(-\theta,-\sigma_1,-\sigma_2) \ , \tag{82}$$

which on substituting into Eq. (72) yields the new general form

$$a(\theta,\sigma_1,\sigma_2) = 2\pi\delta(\theta)a^{(0)}_{\sigma_1\sigma_2} + a_i(\theta,\sigma_1,\sigma_2) \tag{83}$$

$$a_i(\theta,\sigma_1,\sigma_2) = a_c(\theta,\sigma_1,\sigma_2) + \sum_{k=1}^{L}(a^{(k)}_{\sigma_1\sigma_2}\delta(\theta-\theta_k) + a^{(k)}_{-\sigma_1-\sigma_2}\delta(\theta+\theta_k)) \ , \tag{84}$$

where $a^{(k)}$ and a_c are of the general form (80), with $a^{(0)}$ and a_c satisfying as well the additional condition (82). In the case of a_c, this says simply that A and B are even functions of θ, while R and I are odd. (Positivity places no extra constraint on $a^{(k)}$ since $a^{(k)}_{-i-j}$ is automatically positive if $a^{(k)}_{ij}$ is.)

For the constant component $a^{(0)}$ of the transfer matrix, a straightforward generalization of Eq.(55), which we derived for the Schrödinger process, provides immediately a family of options:

$$a^{(0)}(\sigma_1,\sigma_2) = p^*(\sigma_1)p(\sigma_2) \ , \tag{85}$$

with $p(-1)=p(1)=p$, $p(0)=1-2p$, and p any complex number. In this case, the variable part a_i of the transfer matrix can be identified with the interaction term discussed in Section 3.1.

In conclusion, we have the following theorem:

Theorem 6 *Given a fixed positive hermitian matrix $a^{(0)}$ whose components sum to unity, any transfer matrix whose Fourier transform has the form (72), (73), (80), subject to the inequalities (79), gives rise to a strongly positive decoherence functional. Furthermore, if the Fourier transform has the more restrictive form (83), (84), with $a^{(0)}(\sigma_1,\sigma_2) = a^{(0)}(-\sigma_1,-\sigma_2)$ and with A and B even and R and I odd in a_c, then the corresponding quantal random walk is without drift.*

4.2 A simple example

Since we introduced the example of the "non-interacting Schrödinger process" in subsection 3.1 and argued that the type of quantal random walk of greatest interest would be a perturbation of it, we will use such a perturbation to illustrate the general solution just found.

Thus, we take $a^{(0)}$ to be given by Eq. (55), where p is the parameter introduced in Eq. (50). For simplicity, let us choose a solution without drift of the type (84), with $a_c = 0$, $L = 1$, and

$$a^{(1)}(i,j) = \pi p^2 \begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix} . \tag{86}$$

The resulting transfer matrix,

$$a(n_1, \sigma_1, n_2, \sigma_2) = \begin{pmatrix} p^2[1 + \cos((n_2 - n_1)\theta_1)] & -p(2p+i) & p^2[1 - \cos((n_2 - n_1)\theta_1)] \\ -p(2p-i) & 1 + 4p^2 & -p(2p-i) \\ p^2[1 - \cos((n_2 - n_1)\theta_1)] & -p(2p+i) & p^2[1 + \cos((n_2 - n_1)\theta_1)] \end{pmatrix} \tag{87}$$

defines a strongly positive decoherence functional and a quantal measure through Eq. (29). It is particularly simple for $\theta_1 = \pi$, being periodic with period 2 in $n_2 - n_1$.

5 Conclusion

It is noteworthy that one is led to go beyond unitary quantum mechanics in order to arrive at a quantal analog of the random walk. In the wider framework we have implemented in this paper (that of "quantum measure theory" or "generalized quantum theory") unitarity is relinquished but a positivity requirement is retained, as described in detail above. The resulting dynamics furnishes an interesting example of a quantal process belonging to this more general framework.

The family of transfer matrices a derived in Sections 3 and 4 is essentially the most general possible in this framework, for a discrete-time, homogeneous and isotropic random walk on the integers with nearest neighbor transitions and no memory. In addition to these conditions, the only further input to our derivation was the requirement that the transfer matrix a be positive. As we saw, this implies strong positivity of the decoherence functional D and *a fortiori* positivity of the quantum measure μ, i.e. the inequality (16).

We do not believe there is much room for weakening these positivity conditions. Since positivity of the transfer matrix is sufficient and almost certainly necessary for strong positivity of D, the only real question is whether one might consider weakening the latter to weak positivity (16); but it is not clear how much more generality that would achieve, while on the other hand there are good independent reasons for imposing strong positivity in its own right (two such being the consequent existence of a Hilbert space and the guarantee that mentally combining two non-interacting subsystems into a single system will not ruin positivity[13]).

As we have seen, positivity has proven to be remarkably restrictive, and we have been able to find the most general possible transfer matrix that satisfies it. Nevertheless, the resulting random walk still has more free parameters than are present classically, where the homogeneous,

[13] In this way, strong positivity is the analog of what, in another context, is called "complete positivity" for the evolution in time of a quantum mechanical density operator [19].

isotropic walks with step size less than or equal to 1 can be parameterized by a single real number, as in Eq. (69). In contrast, our general transfer matrix contains two even and two odd real *functions*.

An obviously important question is whether some instance of our scheme admits a unitary continuum limit[14]. To a large degree, this seems to be equivalent to asking whether the "interaction" between the paths γ_1 and γ_2 can be chosen so as to reduce in the limit to a final delta function, as in equation (12) or (53); for such a delta-function interaction, were it exact, would immediately imply unitarity of the transfer matrix. If one can come up with an interaction term that does this, then as a consequence a quantal "law of large numbers" should take effect, or at least this seems very plausible. In fact, the Markov property should produce in the continuum limit a differential equation of first order in time, while the locality of the walk (bounded step size) should also imply a differential equation in space. On dimensional grounds[15], the surviving terms in the continuum limit would then be those of lowest possible differential order, namely those of the Schrödinger equation. This would be in close analogy to how the diffusion equation emerges as the continuum limit of the random walk in the classical setting.

To get this kind of delta function behavior one would want the interaction term a_i in (84) to be suitably "attractive". The parameterization we adopted for the transfer matrix in Section 4.1 was chosen with this possibility of a Schrödinger limit in mind, and specifically with the hope that the desired interaction terms would appear as mild perturbations in this parameterization. (Logically speaking however, if there is in fact a "quantal central limit theorem", it would be enough to find any interaction that reduced to a δ-function, using any parameterization.) Based on a preliminary investigation of these issues, we believe the main difficulty in finding an interaction of the desired sort is tied up with the positivity conditions. As we have seen, the "Markov sum rule" (32) implies that the 'interaction part' of the transfer matrix has a nonzero kernel. But this means one is always on the verge of ruining positivity, and one is not free to introduce whatever interaction one wishes. We hope to return to these questions in a future work.

It seems appropriate to conclude this paper with some comments on the physical interpretation of the quantal processes we have defined herein. Obviously, we cannot say anything definitive here because the interpretation of quantum mechanics itself is still not settled. Indeed, the concepts of decoherence functional and quantal measure were introduced in part in the hope of making progress on precisely these interpretational issues by avoiding the invocation of undefined 'measurements' carried out by external agents inhabiting an external, classical world or "laboratory".

At least two interpretive schemes have emerged from these efforts, neither of which is completely worked out yet. Both schemes seek to endow the quantal measure μ with an *intrinsic* meaning that does not need to refer to any external agents at all. The first, and presently more complete scheme aims in effect to realize Bohr's "classical world" within the quantal world by identifying it with a set of decohering variables [11, 20]. Within this scheme, μ would be interpreted as an ordinary probability, but only after restriction to a suitable subset $\mathcal{R}' \subset \mathcal{R}$, namely a subset for which this interpretation would be consistent because all the interference terms $I(A, B)$ would vanish between members of $\mathcal{R}'$ ("decoherence"). Adapting this scheme to

[14]This question is also very relevant for quantum gravity, for reasons given in the Introduction.

[15]Or, if you like, arguing from a gradient expansion, as is done in the context of the "renormalization group".

our quantal random walk, one might, for example, take for A the set of all paths which ever return to the origin and ask whether A decoheres with its complement (call it B). If it did, then one could potentially interpret $\mu(A)$ and $\mu(B) = 1 - \mu(A)$ as probabilities in the normal sense. (Incidentally, if $\mu(B) = 0$, as one might expect, then $I(A, B) = 0$ would follow immediately from strong positivity and Theorem 2.)

The second intrinsic scheme does not demand decoherence and does not attempt to equate μ to a classical probability. Instead, it seeks inspiration from a different feature of the measurement process as it is usually conceived, namely the establishment of a correlation between subsystem and apparatus. It aims to formulate this notion of correlation intrinsically, and it takes such correlations to be objective features of the world which are predictable in terms of the measure μ [13]. Clearly, this scheme could not apply to our random walk *per se*, because there is nothing for the walker to correlate with. One would need to add something like a second walker, or at a minimum some finite-state "meter" which could correlate with some attribute of the walker's trajectory. Beginning with the simplest possibility, one might seek to introduce a second subsystem with trivial internal dynamics, but coupled momentarily to the walker in such a way as to become correlated with some position variable of interest. The enlarged system would again be described by a quantal measure μ' and decoherence functional D', and one could again require strong positivity of the latter. The question then would be under what circumstances such a coupling was possible. (Notice that the original measure μ would play its role indirectly here, by influencing the possible couplings, consistent with strong positivity.) An intriguing question of this sort is whether one could design a "did it ever return?" meter in this manner.

Of course, one could also consider the random walks derived herein more along traditional lines, more in the spirit of the "Copenhagen interpretation", which *does* invoke external observers or instruments to which the rules of classical probability theory are assumed to apply simply by fiat. The nature of such observers is inherently undefined, of course, but the "von Neumann scheme" permits them to be modeled as quantum systems, at the cost of having to introduce some still more primitive external agents to measure the measurers. Because it is logically circular, this process of "moving the cut" does not really explain the measurement process, but it does establish a certain self consistency of the textbook measurement paradigm. One could try to formulate an analogous "measurement theory" for generalized quantum mechanics (in terms of D and μ rather than the state-vector) and apply it to our random walk. This could mean figuring out how to couple an effectively classical "apparatus" to, e.g., the walker's position at a certain time. Since different positions of the walker will not in general decohere in our case, no classical apparatus could be expected to reproduce the quantal measure of a "position predicate" directly as the probability of a meter reading. (That is why the "consistent historians" demand decoherence in the first place, of course.) Hence, to make the scheme go through in its familiar form, one would have to find other variables that did in fact decohere, and therefore "could be measured".

Alternatively, one might seek a "self consistent" measurement model that invoked external agents, but did not try to reduce quantal measures to classical ones (probabilities). In other words, one would allow "meter readings" to interfere, and would seek to couple the quantal walker to a quantal meter in such a way that the quantal measure of a given meter reading after coupling would coincide with the quantal measure of the corresponding set of walker trajectories in the uncoupled case. This would be more completely parallel to the usual paradigm in the sense that it would exhibit the self consistency of this sort of "measurement", without shedding any further light on the meaning of D or μ as such.

A rather different way to seek an interpretation of our quantal random walk would be to ask whether one could *realize* it using ordinary unitary processes (see [21] for a related discussion). Could one, for example, simulate it on a computer? We suspect that this would be impossible with a classical computer, but it might be possible with a quantum one. Since our random walk is not unitary, it could only be realized, within a unitary framework, as an open system (or more generally an incomplete set of variables). Could one, then, program a quantum computer so that its decoherence functional would reproduce that of the random walk when restricted to a suitable set of discrete variables? (In addressing this question, the affinity between strong and complete positivity might be helpful, since it is known that any completely positive dynamics can be reproduced as the effective dynamics of a subsystem of a larger unitary system.)

Thus, there remain many open questions for the future, whose investigation promises to yield further insight into the quantum world.

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