

Classical and Quantum Propagation of Chaos

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1 Overview

The concept of molecular chaos dates back to Boltzmann [3], who derived the fundamental equation of the kinetic theory of gases under the hypothesis that the molecules of a nonequilibrium gas are in a state of “molecular disorder.” The concept of *propagation* of molecular chaos is due to Kac [8, 9], who called it “propagation of the Boltzmann property” and used it to derive the homogeneous Boltzmann equation in the infinite-particle limit of certain Markovian gas models (see also [5, 17]). McKean [12, 13] proved the propagation of chaos for systems of interacting diffusions that yield diffusive Vlasov equations in the mean-field limit. Spohn [16] used a quantum analog of the propagation of chaos to derive time-dependent Hartree equations for mean-field Hamiltonians, and his work was extended in [1] to open quantum mean-field systems.

This article examines the relationship between classical and quantum propagation of chaos. The rest of this introduction reviews some ideas of quantum probability and dynamics. Section 2 discusses the classical and quantum concepts of propagation of chaos. In Section 3, *classical* propagation of chaos is shown to occur when *quantum* systems that propagate quantum molecular chaos are suitably prepared, allowed to evolve without interference, and then observed. Our main result is Corollary 3.7, which may be paraphrased as follows:

Let \mathcal{O} be a complete observable of a single particle, taking its values in a countable set J , and let \mathcal{O}_i denote the observable \mathcal{O} of particle i in a system of n distinguishable particles of the same species. Suppose we allow that quantum n -particle system to evolve freely, except that we periodically measure $\mathcal{O}_1, \mathcal{O}_2, \dots, \mathcal{O}_n$. The resulting time series of measurements is a Markov chain

in J^n . If the sequence of n -particle dynamics propagates quantum molecular chaos, then these derived Markov chains propagate chaos in the classical sense.

Results like this may be of interest to probabilists who already know some examples of the propagation of chaos and who may be surprised to learn of novel examples arising in quantum dynamics. An effort has been made here to expound the propagation of quantum molecular chaos for such an audience, while the classical propagation of chaos *per se* is discussed only briefly in Section 2.1. The reader is referred to [18] and [14] for two definitive surveys of the classical propagation of chaos.

1.1 Quantum kinematics

In quantum theory, the state of a physical system is inherently statistical: the state of a system \mathcal{S} does not *determine* whether or not \mathcal{S} has a given property, but rather, the state provides only the *probability* that \mathcal{S} would be found to have that property, if we were to check for it. The properties that \mathcal{S} might or might not have are represented by orthogonal projectors on some Hilbert space. If a projector P represents a property P of \mathcal{S} , then the complementary property NOT P is represented by $I - P$. The identity and zero operators I and $\mathbf{0}$ represent the trivial properties TRUE and FALSE respectively. If P and Q are properties whose orthogonal projectors are P and Q , the properties (P AND Q) and (P OR Q) are defined if and only if P and Q commute, in which case $PQ = QP$ represents (P AND Q) and $P + Q - PQ$ represents (P OR Q). A countable *resolution of the identity* is a countable family of projectors $\{P_j\}$ such that

$$P_j P_{j'} = P_{j'} P_j = \mathbf{0}; \quad \forall j \neq j'$$

and $I = \sum_j P_j$. This represents a partition of the space of outcomes of a measurement on \mathcal{S} into a countable set of elemental properties, which are mutually exclusive and collectively exhaustive. A *state* ω of the system \mathcal{S} is a function that assigns probabilities to the properties of \mathcal{S} , or their projections. Thus we suppose that $\omega(I) = 1$, $\omega(\mathbf{0}) = 0$ and also that

$$\omega(I - P) + \omega(P) = \omega(I) = 1.$$

Indeed, it is rational to suppose that any state ω must satisfy

$$1 = \omega(I) = \omega\left(\sum_j P_j\right) = \sum_j \omega(P_j) \quad (1)$$

for any countable resolution of the identity $\{P_j\}$.

Having made these introductory comments, we revert to a more technical description of the mathematical set-up. Suppose the properties of a quantum system \mathcal{S} are represented by orthogonal projectors in $\mathcal{B}(\mathbb{H})$, the bounded operators on a Hilbert space \mathbb{H} . The *statistical states* (also called simply *states*) of that quantum system are identified with the normal positive linear functionals on $\mathcal{B}(\mathbb{H})$ that assign 1 to the identity operator. A positive linear functional ω on $\mathcal{B}(\mathbb{H})$ is *normal* if

$$\sum_{a \in A} \omega(P_a) = 1$$

whenever $\{P_a\}_{a \in A}$ is a family of commuting projectors that sum to the identity operator (i.e., the net of finite partial sums of the projectors converges in the weak operator topology to the identity). Normal states are in one-one correspondence with *density operators*, positive trace-class operators of trace 1. If D is a density operator on \mathbb{H} then $A \mapsto \text{Tr}(DA)$ defines a normal state on $\mathcal{B}(\mathbb{H})$; conversely, every normal state ω on $\mathcal{B}(\mathbb{H})$ is of the form $\omega(A) = \text{Tr}(DA)$ for some density operator D . The density operators form a closed convex subset of the trace-class operators, which is a Banach space with $\|T\| = \text{Tr}(|T|)$. The dual of the Banach space of trace class operators is $\mathcal{B}(\mathbb{H})$ with its operator norm.

In the Heisenberg picture of quantum dynamics — where the state is constant while the operators corresponding to observables change — the dynamics are given by unitarily implemented automorphisms of the bounded operators on a Hilbert space. That is, for each $\tau \geq 0$ there exists a unitary operator $U(\tau)$ such that a property represented by P at time $t = 0$ is represented by

$$P(\tau) = U(\tau)^* P U(\tau) \tag{2}$$

at time $t = \tau$. In the Schrödinger picture of dynamics, the density operator D of the quantum state changes in time while the projectors P that represent properties of the system remain fixed. The Schrödinger formulation of the dynamics corresponding to (2) is

$$D(\tau) = U(\tau) D(0) U(\tau)^*,$$

because, for any $P \in \mathcal{B}(\mathbb{H})$,

$$\text{Tr}[D P(\tau)] = \text{Tr}[D U(\tau)^* P U(\tau)] = \text{Tr}[U(\tau) D U(\tau)^* P] = \text{Tr}[D(\tau) P].$$

The Heisenberg picture of dynamics suggests a generalization where the dynamics $A \mapsto U^*AU$ are replaced by more general endomorphisms of $\mathcal{B}(\mathbb{H})$, namely, by completely positive maps $\phi : \mathcal{B}(\mathbb{H}) \rightarrow \mathcal{B}(\mathbb{H})$ such that $\phi(I) = I$. These endomorphisms include the automorphisms $A \mapsto U^*AU$ of the Heisenberg picture of quantum dynamics, but also describe maps of observables $A \mapsto \phi(A)$ effected by the intervention of measurements, randomization, and coupling to other systems. A map ϕ is positive if it maps nonnegative operators to nonnegative operators, and it is *completely positive* if $\phi \otimes \text{id}_d$ is positive whenever id_d is the identity on $\mathcal{B}(\mathbb{C}^d)$ for any finite d . Requiring ϕ to be positive and unital (unit preserving) is necessary to ensure that (1) holds, at least for any finite resolution of the identity. The *complete* positivity of ϕ ensures the positivity of the dynamics of certain extensions of the original system \mathcal{S} , where \mathcal{S} is considered together with a physically independent, finite-dimensional quantum system. To pass to the Schrödinger picture we must impose the further technical requirement that the map ϕ be *normal*, i.e., ϕ is assumed to be such that

$$\lim \phi(A_\alpha) = \phi(A)$$

whenever $\{A_\alpha\}$ is a monotone increasing net of positive operators with least upper bound A . This way the Schrödinger dynamics of the normal state can be defined as the “predual” of the Heisenberg dynamics; if ϕ is normal then the relation

$$\text{Tr}(\phi_*(D)A) = \text{Tr}(D\phi(A)) \quad \forall A \in \mathcal{B}(\mathbb{H})$$

implicitly defines a trace-preserving map ϕ_* known as the *predual* of ϕ . In the Schrödinger picture, the density operator D that describes the quantum state undergoes the transformation $D \mapsto \phi_*(D)$, where ϕ is a normal completely positive unital endomorphism of $\mathcal{B}(\mathbb{H})$.

The description of a quantum system evolving continuously in time requires a normal and completely positive endomorphism of $\mathcal{B}(\mathbb{H})$ for each $t > 0$, to describe the change of observables (in the Heisenberg picture) from time 0 to time t . A *quantum dynamical semigroup*, or QDS, is a family $\{\phi_t\}_{t \geq 0}$ of normal completely positive (and unital) endomorphisms of the bounded operators on some Hilbert space \mathbb{H} , which is a semigroup (i.e., $\phi_0 = \text{id}$ and $\phi_t \circ \phi_s = \phi_{t+s}$ for $s, t \geq 0$) and which has weak*-continuous trajectories: for any $B \in \mathcal{B}(\mathbb{H})$ and any trace class operator T

$$\text{Tr}(T \phi_t(B))$$

is continuous in t . (We will not need the continuity of trajectories in this article.) Quantum dynamical semigroups describe the continuous change of the state of an open quantum system whose dynamics are autonomous and Markovian. Many models of open quantum systems are QDSs (but not all, viz. [10]). We will use the notation $(\phi)_t$ for the whole QDS:

$$(\phi)_t = \{\phi_t\}_{t \geq 0}. \quad (3)$$

2 Classical and Quantum Molecular Chaos

2.1 Classical molecular chaos

Molecular chaos is a type of stochastic independence of particles manifesting itself in an infinite-particle limit.

Let Ω^n be the n -fold Cartesian power of a measurable space Ω . A probability measure p on Ω^n is called *symmetric* if

$$p(E_1 \times E_2 \times \cdots \times E_n) = p(E_{\pi(1)} \times E_{\pi(2)} \times \cdots \times E_{\pi(n)})$$

for all measurable sets $E_1, \dots, E_n \subset \Omega$ and all permutations π of $\{1, 2, \dots, n\}$. For $k \leq n$, the k -*marginal* of p , denoted $p^{(k)}$, is the probability measure on S^k satisfying

$$p^{(k)}(E_1 \times E_2 \times \cdots \times E_k) = p(E_1 \times \cdots \times E_k \times \Omega \times \cdots \times \Omega)$$

for all measurable sets $E_1, \dots, E_k \subset \Omega$. In the context of classical probability theory, one defines molecular chaos as follows [18]:

Definition 2.1. Let Ω be a separable metric space. Let p be a probability measure on Ω , and for each $n \in \mathbb{N}$, let p_n be a symmetric probability measure on Ω^n .

The sequence $\{p_n\}$ is **p -chaotic** if the k -marginals $p_n^{(k)}$ converge weakly to $p^{\otimes k}$ as $n \rightarrow \infty$, for each fixed $k \in \mathbb{N}$.

A sequence, indexed by n , of n -particle dynamics *propagates chaos* if molecularly chaotic sequences of initial distributions remain molecularly chaotic for all time under the n -particle dynamical evolutions. In the classical contexts [9, 12, 14, 18] the dynamics are Markovian and the state spaces are usually taken to be separable and metrizable. Accordingly, in my dissertation [4] I defined propagation of chaos in terms of Markov transition kernels, as follows:

Definition 2.2 (Classical Propagation of Chaos). Let Ω be a separable metric space. For each $n \in \mathbb{N}$, let $K_n : \Omega^n \times \sigma(\Omega^n) \rightarrow [0, 1]$ be a Markov transition kernel which is invariant under permutations in the sense that

$$K_n(\mathbf{x}, E) = K_n(\pi \cdot \mathbf{x}, \pi \cdot E)$$

for all permutations π of the n coordinates of \mathbf{x} and the points of $E \subset \Omega^n$. Here, $\sigma(\Omega^n)$ denotes the Borel σ -field of Ω^n .

The sequence $\{K_n\}_{n=1}^\infty$ **propagates chaos** if the molecular chaos of a sequence $\{p_n\}$ entails the molecular chaos of the sequence

$$\left\{ \int_{\Omega^n} K_n(\mathbf{x}, \cdot) p_n(d\mathbf{x}) \right\}_{n=1}^\infty. \quad (4)$$

The preceding formulation of the propagation of molecular chaos is technically straightforward but not flexible enough to cover the weaker kinds of propagation of chaos phenomena that occur in several applications, most notably in the landmark derivation of the Boltzmann equation due to Lanford and King [11]. Nonetheless, it is still worthwhile to make Definition 2.2. Those models that exhibit weak propagation of chaos phenomena usually have less realistic regularizations that propagate molecular chaos in the sense of Definition 2.2. Moreover, this definition has the pleasant feature that it implies that $\{K_n \circ L_n\}$ propagates molecular chaos when $\{K_n\}$ and $\{L_n\}$ do.

2.2 Quantum molecular chaos

The Hilbert space of pure states of a collection of n distinguishable components is $\mathbb{H}_1 \otimes \cdots \otimes \mathbb{H}_n$, where \mathbb{H}_i is the Hilbert space for the i^{th} component. The Hilbert space for n distinguishable components of the same species will be denoted $\mathbb{H}^{\otimes n}$. If D_n is a density operator on $\mathbb{H}^{\otimes n}$, then its k -marginal, or partial trace, is a density operator on $\mathbb{H}^{\otimes k}$ that gives the statistical state of the first k particles. The k -marginal may be denoted $\text{Tr}^{(n-k)} D_n$ and defined as follows: Let O be any orthonormal basis of \mathbb{H} . If $x \in \mathbb{H}^{\otimes k}$ with $k < n$ then for any $w, x \in \mathbb{H}^{\otimes k}$

$$\begin{aligned} \left\langle \text{Tr}^{(n-k)} D_n(w), x \right\rangle &= \\ \sum_{y_1, \dots, y_{n-k} \in O} \left\langle D_n(w \otimes y_1 \otimes \cdots \otimes y_{n-k}), x \otimes y_1 \otimes \cdots \otimes y_{n-k} \right\rangle. \end{aligned}$$

A linear functional ω on $\mathcal{B}(\mathbb{H}^{\otimes n})$ is *symmetric* if it satisfies

$$\omega(A_1 \otimes \cdots \otimes A_n) = \omega(A_{\pi(1)} \otimes A_{\pi(2)} \otimes \cdots \otimes A_{\pi(n)})$$

for all permutations π of $\{1, 2, \dots, n\}$ and all $A_1, \dots, A_n \in \mathcal{B}(\mathbb{H})$. For each permutation π of $\{1, 2, \dots, n\}$, define the unitary operator U_π on $\mathbb{H}^{\otimes n}$ whose action on simple tensors is

$$U_\pi(x_1 \otimes x_2 \otimes \cdots \otimes x_n) = x_{\pi(1)} \otimes x_{\pi(2)} \otimes \cdots \otimes x_{\pi(n)}. \quad (5)$$

A density operator D_n represents a symmetric functional on $\mathcal{B}(\mathbb{H}^{\otimes n})$ if and only if D_n commutes with each U_π . Two special types of symmetric density operators are Fermi-Dirac densities, which represent the statistical states of systems of fermions, and Bose-Einstein densities, which represent the statistical states of systems of bosons. Bose-Einstein density operators are characterized by the condition that $D_n U_\pi = D_n$ for all permutations π , and Fermi-Dirac densities are characterized by the condition that $D_n U_\pi = \text{sign}(\pi) D_n$ for all π .

To recapitulate, n -component states are given by density operators on $\mathbb{H}^{\otimes n}$ and, in the Schrödinger picture, the dynamics transforms an initial state $A \mapsto \text{Tr}(DA)$ into a state of the form $A \mapsto \text{Tr}(D\phi(A))$, where ϕ is a normal completely positive unital endomorphism of $\mathcal{B}(\mathbb{H}^{\otimes n})$. This is the context of the following two definitions:

Definition 2.3. Let D be a density operator on \mathbb{H} , and for each $n \in \mathbb{N}$, let D_n be a symmetric density operator on $\mathbb{H}^{\otimes n}$.

The sequence $\{D_n\}$ is **D -chaotic in the quantum sense** if, for each fixed $k \in \mathbb{N}$, the density operators $\text{Tr}^{(n-k)} D_n$ converge in trace norm to $D^{\otimes k}$ as $n \rightarrow \infty$.

The sequence $\{D_n\}$ is **quantum molecularly chaotic** if it is D -chaotic in the quantum sense for some density operator D on \mathbb{H} .

The definitions of classical and quantum molecular chaos are somewhat incongruous. This definition of quantum molecular chaos requires that the marginals converge in the trace norm, whereas the notion of classical molecular chaos used in Probability Theory requires *weak* convergence of the marginals. In fact, Definition 2.1 of classical molecular chaos and the “commutative” version of Definition 2.3 (obtained by extending that definition of quantum molecular chaos to commutative von Neumann algebras) are not

equivalent! Nonetheless, I have chosen Definition 2.3 because the attractive theory of quantum mean-field kinetics presented in Section 2.3 favors a formulation of quantum molecular chaos in terms of the trace norm.

Definition 2.4 (Propagation of Quantum Molecular Chaos). For each $n \in \mathbb{N}$, let ϕ_n be a normal completely positive map from $\mathbb{H}^{\otimes n}$ to itself that fixes the identity and which commutes with permutations, i.e., such that

$$\phi_n(U_\pi^* A U_\pi) = U_\pi^* \phi_n(A) U_\pi \quad (6)$$

for all $A \in \mathcal{B}(\mathbb{H}^{\otimes n})$ and all permutations π of $\{1, 2, \dots, n\}$, where U_π is as defined in (5).

The sequence $\{\phi_n\}$ **propagates quantum molecular chaos** if the quantum molecular chaos of a sequence of density operators $\{D_n\}$ entails the quantum molecular chaos of the sequence $\{\phi_{n*}(D_n)\}$.

We shall soon find that there are interesting examples of quantum dynamical semigroups $(\phi_n)_t$ with the collective property that $\{\phi_{n,t}\}$ propagates quantum molecular chaos for each fixed $t > 0$. When this happens, it is convenient to say that the sequence $\{(\phi_n)_t\}$ of QDSs propagates chaos.

Definition 2.5. For each n let $(\phi_n)_t$ be a QDS on $\mathcal{B}(\mathbb{H}^{\otimes n})$ that satisfies the permutation condition (6). The sequence $\{(\phi_n)_t\}$ **propagates molecular chaos** if $\{\phi_{n,t}\}$ propagates quantum molecular chaos for every fixed $t > 0$.

2.3 Spohn's quantum mean-field dynamics

There are several successful mathematical treatments of quantum mean-field dynamics. One of them, due to H. Spohn, relies upon the concept of propagation of quantum molecular chaos. Spohn's theorem [16] constitutes a rigorous derivation of the time-dependent Hartree equation for bounded mean-field potentials.

Let V be a bounded Hermitian operator on $\mathbb{H} \otimes \mathbb{H}$ such that $VU_{(12)} = U_{(12)}V(y \otimes x)$, representing a symmetric two-body potential. Let $V_{1,2}$ denote the operator on $\mathbb{H}^{\otimes n}$ defined by

$$V_{1,2}(x_1 \otimes x_2 \otimes \cdots \otimes x_n) = V(x_1 \otimes x_2) \otimes x_3 \otimes \cdots \otimes x_n, \quad (7)$$

and for each $i, j \leq n$ with $i < j$, define V_{ij} similarly, so that it acts on the i^{th} and j^{th} factors of each simple tensor. This may be accomplished by setting

$V_{ij} = U_\pi^* V_{1,2} U_\pi$, where $\pi = (2j)(1i)$ is a permutation that puts i in the first place and j in the second place, and U_π is as defined in (5). Define the n -particle Hamiltonians H_n as the sum of the pair potentials V_{ij} , with common coupling constant $1/n$:

$$H_n = \frac{1}{n} \sum_{i < j} V_{ij}. \quad (8)$$

If D_n is a state on $\mathbb{H}^{\otimes n}$, let $D_n(t)$ denote the state of an n -particle system that was initially in state D_n and which has undergone t units of the temporal evolution governed by the Hamiltonian (8):

$$D_n(t) = e^{-iH_n t/\hbar} D_n e^{iH_n t/\hbar}. \quad (9)$$

Theorem 2.6 (Spohn). *Suppose D is a density operator on \mathbb{H} and $\{D_n\}$ is a D -chaotic sequence of symmetric density operators on $\mathbb{H}^{\otimes n}$. Then the sequence of density operators $\{D_n(t)\}$ defined in (8) and (9) is $D(t)$ -chaotic, where $D(t)$ is the solution at time t of the following initial-value problem in the Banach space of trace-class operators:*

$$\begin{aligned} \frac{d}{dt} D(t) &= -\frac{i}{\hbar} \text{Tr}^{(n-1)}[V, D(t) \otimes D(t)] \\ D(0) &= D. \end{aligned} \quad (10)$$

In other words, if H_n is as in (8) and $\phi_n(A) = e^{iH_n t/\hbar} A e^{-iH_n t/\hbar}$ then the sequence $\{\phi_n\}$ propagates quantum molecular chaos. See [16] for a short proof.

It must be emphasized that the preceding approach does not apply to systems of Fermions. In other words, Theorem 2.6 yields time-dependent Hartree equations but not time-dependent Hartree-Fock equations (which include an exchange term that enforces the Pauli Principle). The problem is that there exists no molecularly chaotic sequence of Fermi-Dirac states because the antisymmetry of Fermi-Dirac states is incompatible with the factorization of molecularly chaotic states. To derive time-dependent Hartree-Fock equations despite this problem is a goal of current research [15].

Spohn's approach can be generalized to handle Hamiltonians which involve the usual unbounded kinetic energy operators, and to handle *open* quantum mean-field systems. In [1], Theorem 2.6 is extended to systems where the free motion of the single particle may have an unbounded self-adjoint generator and the two-particle generator may have the Lindblad form. The "propagation of quantum molecular chaos" is called the "mean-field property" in that article.

3 Classical Manifestations of the Propagation of Quantum Molecular Chaos

A sequence $\{\phi_n\}$ that propagates quantum molecular chaos mediates a variety of instances of the propagation of classical molecular chaos.

Given a D -chaotic sequence of density operators $\{D_n\}$ one can produce a variety of molecularly chaotic sequences $\{q_n\}$ of probability measures. For each single-particle measurement \mathcal{M} , the joint probabilities q_n of the outcome of applying \mathcal{M} to all of the particles form a molecularly chaotic sequence. Conversely, there are ways to convert a p -chaotic sequence $\{p_n\}$ of probability measures into a D -chaotic sequence of density operators $\{D_n\}$. Suppose we are presented with a sequence of quantum dynamics $\{\phi_n\}$ that propagates quantum molecular chaos. We can first *encode* a sequence of molecularly chaotic probabilities $\{p_n\}$ as a quantum molecularly chaotic sequence of density operators $\{D_n\}$, then allow $\{D_n\}$ to *develop* into a new sequence $\{\phi_{n*}(D_n)\}$ under the dynamics, and finally *read* the resulting quantum states by applying some single-particle measurement to each of the particles. This procedure converts one molecularly-chaotic sequence of probability measures into another, i.e., it propagates chaos in the classical sense.

The next three sections examine the encode/develop/read-procedure that converts quantum molecular chaos to classical molecular chaos. Finally, in Section 3.4, we show how to produce Markov chains that propagate chaos by observing quantum processes that propagate chaos.

3.1 Generalized measurements and the reading procedure

Let \mathbb{H} be a Hilbert space and (Ω, \mathcal{F}) a measurable space. A *positive operator valued measure*, or POVM, is a function $X(E)$ from \mathcal{F} to the positive operators on \mathbb{H} which is countably additive with respect to the weak operator topology:

$$\sum_{i=1}^{\infty} X(E_i) = X(E)$$

in the weak operator topology whenever the sets $E_i \in \mathcal{F}$ are disjoint and $E = \cup E_i$. In the special case that the positive operators $X(E)$ are self-adjoint projections such that $X(E)X(F) = \mathbf{0}$ when $E \cap F = \emptyset$, the POVM

is just a resolution of identity on (Ω, \mathcal{F}) . A POVM defines an affine map $D \mapsto p_{D,X}$ from density operators on \mathbb{H} to probability measures on Ω . For any density operator D ,

$$p_{D,X}(\cdot) = \text{Tr}[DX(\cdot)] \quad (11)$$

is a countably additive probability measure on (Ω, \mathcal{F}) .

POVMs correspond to *generalized* Ω -valued measurements just as the spectral decomposition of a self-adjoint operator corresponds to a simple measurement. A generalized measurement is realized by performing a simple measurement on a composite system consisting of the system of interest and an “ancillary system” that has been prepared to have state E , without allowing any interaction between the system itself and the ancillary system or the environment. Suppose that \mathbb{H}_a is the Hilbert space of an ancillary space that has been prepared in state E , and $P(d\omega), \omega \in \Omega$ is the spectral measure belonging to an observable \mathcal{O} on the composite system $\mathbb{H} \otimes \mathbb{H}_a$. If the system of interest is in state D when \mathcal{O} is measured, a random $\omega \in \Omega$ is produced, governed by the probability law $\text{Tr}[(D \otimes E) P(d\omega)]$. This probability law has the form (11), since

$$\text{Tr}[(D \otimes E) P(d\omega)] = \text{Tr}[D \text{Tr}^{(1)}((I \otimes E)P(d\omega))] = \text{Tr}(DX(d\omega))$$

where $X(d\omega)$ is the POVM

$$X(d\omega) = \text{Tr}^{(1)}((I \otimes E^{1/2})P(d\omega)(I \otimes E^{1/2})).$$

This shows that the outcome of a generalized measurement is governed by some POVM as in (11). Conversely, it can be shown that any POVM arises in this way from some conceivable (but perhaps impracticable) generalized measurement of the type we have just described [7].

The following lemma has a straightforward proof, which we omit.

Lemma 3.1. *Let Ω be a separable metric space with Borel σ -field $\sigma(\Omega)$, and let $X : \sigma(\Omega) \rightarrow \mathcal{B}(\mathbb{H})$ be a POVM on Ω .*

For each n , let D_n be a symmetric density operator on $\mathcal{B}(\mathbb{H}^{\otimes n})$, and suppose that $\{D_n\}$ is D -chaotic in the quantum sense.

Then the sequence of probability measures $\{p_n\}$ is p -chaotic, p_n and p being defined by

$$\begin{aligned} p(A) &= \text{Tr}(DA) \\ p_n(A_1 \times A_2 \times \cdots \times A_n) &= \text{Tr}(D_n X(A_1) \otimes \cdots \otimes X(A_n)). \end{aligned}$$

3.2 Lemmas concerning the encoding procedure

The procedure for encoding probability measures as density operators depends on our choice of a density operator valued function $D(\omega)$ on the single-particle space Ω , now assumed to be a separable metric space. Let us choose a function $D(\omega)$ from Ω to the density operators on a Hilbert space \mathbb{H} , and assume D is continuous for technical convenience. Then we can convert a probability measure p_n on Ω^n into the density operator

$$\int_{\Omega^n} D(\omega_1) \otimes D(\omega_2) \otimes \cdots \otimes D(\omega_n) p_n(d\omega_1 d\omega_2 \cdots d\omega_n)$$

on $\mathbb{H}^{\otimes n}$. If $\{p_n\}$ is a p -chaotic sequence of symmetric measures on Ω^n then the corresponding sequence of density operators is quantum molecularly chaotic — but only in a weak sense! Think of the density operators as a subset of the Banach space of trace-class operators. Each continuous linear functional on this space has the form

$$T \longmapsto \text{Tr}(TB)$$

where B is a bounded operator, for $\mathcal{B}(\mathbb{H})$ is the Banach dual of the space of trace-class operators on \mathbb{H} . A sequence $\{T_n\}$ of trace-class operators on \mathbb{H} is *weakly convergent* if

$$\lim_{n \rightarrow \infty} \text{Tr}(T_n B) = \text{Tr}(TB)$$

for all $B \in \mathcal{B}(\mathbb{H})$.

Lemma 3.2. *Let Ω be a separable metric space and suppose $\{p_n\}$ is a p -chaotic sequence of symmetric measures on Ω^n . Let $D(s)$ be a continuous function from Ω to the density operators on a Hilbert space \mathbb{H} .*

Define \bar{D} and D_n by

$$\begin{aligned} \bar{D} &= \int_{\Omega} D(\omega) p(d\omega) \\ D_n &= \int_{\Omega^n} D(\omega_1) \otimes D(\omega_2) \otimes \cdots \otimes D(\omega_n) p_n(d\omega_1 d\omega_2 \cdots d\omega_n). \end{aligned} \tag{12}$$

Then, for each k , the sequence of marginals $\{\text{Tr}^{(n-k)} D_n\}$ converges weakly to $\bar{D}^{\otimes k}$ as $n \rightarrow \infty$.

Proof. The integrals in (12) may be defined as Bochner integrals in the Banach space of trace-class operators (see [6] Theorem 3.7.4). The partial trace is a bounded operator from the Banach space of trace-class operators on \mathbb{H}^n to the Banach space of trace-class operators on \mathbb{H}^k , so Theorem 3.7.12 of [6] implies that

$$\begin{aligned} & \mathrm{Tr}^{(n-k)} \int_{\Omega^n} D(\omega_1) \otimes \cdots \otimes D(\omega_n) p_n(d\omega_1 d\omega_2 \cdots d\omega_n) \\ &= \int_{\Omega^n} D(\omega_1) \otimes \cdots \otimes D(\omega_k) p_n(d\omega_1 d\omega_2 \cdots d\omega_n). \end{aligned} \tag{13}$$

Since Bochner integration commutes with application of bounded linear functionals, the right hand side of (13) converges weakly to

$$\int_{\Omega^k} D(\omega_1) \otimes D(\omega_2) \otimes \cdots \otimes D(\omega_k) p^{\otimes k}(d\omega_1 d\omega_2 \cdots d\omega_k) = \bar{D}^{\otimes k}$$

as $n \rightarrow \infty$. □

The preceding lemma does not conclude that $\{D_n\}$ is quantum molecularly chaotic in the sense of our Definition 2.3, which requires convergence of the partial traces in trace norm. Some additional conditions seem necessary in order to conclude that the encoding procedure produces quantum molecular chaos. The easiest thing to do is suppose that the quantum systems involved are finite dimensional. This affords a quick way to construct Markov transitions on any space Ω . The opposite approach is to let the mediating quantum dynamics occur in any Hilbert space \mathbb{H} but to suppose that Ω is discrete. We follow these two approaches in the next two lemmas:

Lemma 3.3. *If \mathbb{H} is a finite dimensional Hilbert space \mathbb{C}^d , and D_n and D are as in the statement of Lemma 3.2, then the sequence of states $\{D_n\}$ is \bar{D} -chaotic.*

Proof. From Lemma 3.2 we know that $\{\mathrm{Tr}^{(n-k)} D_n\}$ converges weakly to $\bar{D}^{\otimes k}$ as $n \rightarrow \infty$. But a sequence of trace-class operators on \mathbb{C}^d converges in trace norm if it converges weakly, since the Banach space of trace class operators on \mathbb{C}^d is finite-dimensional. Hence, $\lim_{n \rightarrow \infty} \mathrm{Tr}^{(n-k)}(D_n) = \bar{D}^{\otimes k}$ in trace norm, as required. □

Now we consider a set J with a discrete topology and σ -field. We note that if the word “separable” were removed from Definition 2.1 of classical molecular chaos then the following lemma would hold even for uncountable sets J :

Lemma 3.4. *Let J be a countable set equipped with the discrete topology and its Borel σ -field (so that every subset of J is measurable), and let $\{D(j)\}_{j \in J}$ be a family of density operators on \mathbb{H} indexed by J .*

Suppose p is a probability measure on J and $\{p_n\}$ is a p -chaotic sequence of probability measures. Define

$$\begin{aligned} \bar{D} &= \sum_{j \in J} p(j) D(j) \\ D_n &= \sum_{(j_1, \dots, j_n) \in J^n} p_n(j_1, \dots, j_n) D(j_1) \otimes D(j_2) \otimes \cdots \otimes D(j_n). \end{aligned} \tag{14}$$

Then $\{D_n\}$ is D -chaotic.

Proof. Since the series defining D_n converges in trace norm and the partial trace operator $\text{Tr}^{(n-k)}$ is a bounded operator with respect to the trace norm, it follows that

$$\begin{aligned} \text{Tr}^{(n-k)} D_n &= \sum_{J^n} p_n(j_1, \dots, j_n) D(j_1) \otimes D(j_2) \otimes \cdots \otimes D(j_k) \\ &= \sum_{J^k} p_n^{(k)}(j_1, \dots, j_k) D(j_1) \otimes D(j_2) \otimes \cdots \otimes D(j_k). \end{aligned}$$

Now $\{p_n^{(k)}\}$ converges weakly to $p^{\otimes k}$ as n tends to infinity, for $\{p_n\}$ is p -chaotic. Since a sequence of elements of ℓ^1 converges in norm if and only if it converges weakly [2], the sequence $\{p_n^{(k)}\}$ converges in the ℓ^1 norm to $p^{\otimes k}$ as n tends to infinity. Hence, in trace norm,

$$\begin{aligned} \lim_{n \rightarrow \infty} \text{Tr}^{(n-k)} D_n &= \sum_{J^k} p(j_1) p(j_2) \cdots p(j_k) D(j_1) \otimes D(j_2) \otimes \cdots \otimes D(j_k) \\ &= \bar{D}^{\otimes k}, \end{aligned}$$

proving that $\{D_n\}$ is \bar{D} -chaotic. \square

3.3 Putting it together: encoding, developing, and reading

We now formulate two abstract propositions that follow from the above two lemmas on the encoding procedure. Proposition 3.5 relies on Lemma 3.3 and is therefore limited by the hypothesis that the mediating quantum system is finite-dimensional. Proposition 3.6 is derived from Lemma 3.4. It allows the quantum dynamics to take place in an arbitrary Hilbert space but requires the measurable spaces involved to be discrete. Despite these technical restrictions there remains a rich variety of classical examples of the propagation of chaos residing within each instance of the propagation of quantum molecular chaos.

Proposition 3.5. *Let Ω be a separable metric space with Borel σ -field $\sigma(\Omega)$, let $D(s)$ be a continuous function from Ω to the density operators on \mathbb{C}^d , and let $X : \sigma(\Omega) \rightarrow \mathcal{B}(\mathbb{C}^d)$ be a POVM on Ω . For each n , let ϕ_n be a normal completely positive unital endomorphism of $\mathcal{B}((\mathbb{C}^d)^{\otimes n})$ that satisfies (6).*

Define the Markov transition kernel K_n on Ω^n by

$$\begin{aligned} K_n((\omega_1, \omega_2, \dots, \omega_n), A_1 \times A_2 \times \dots \times A_n) \\ = \text{Tr} [(D(\omega_1) \otimes \dots \otimes D(\omega_n)) \phi_n(X(A_1) \otimes \dots \otimes X(A_n))]. \end{aligned}$$

If $\{\phi_n\}$ propagates quantum molecular chaos then $\{K_n\}$ propagates molecular chaos in the classical sense.

The proof of this proposition is omitted because it follows directly from Lemma 3.1 and Lemma 3.3. Likewise, the following proposition follows from Lemma 3.1 and Lemma 3.4:

Proposition 3.6. *Let \mathbb{H} be a Hilbert space and, for each n , let ϕ_n be a completely positive endomorphism of $\mathcal{B}(\mathbb{H}^{\otimes n})$ that satisfies (6). Let J be a countable set equipped with the discrete topology and σ -field, and let $X : J \rightarrow \mathcal{B}(\mathbb{H})$ be a POVM on J .*

Define the Markov transition matrices K_n on J^n by

$$\begin{aligned} K_n((j_1, \dots, j_n), (j'_1, \dots, j'_n)) \\ = \text{Tr} [(D(j_1) \otimes \dots \otimes D(j_n)) \phi_n(X(j'_1) \otimes \dots \otimes X(j'_n))] \end{aligned}$$

If $\{\phi_n\}$ propagates quantum molecular chaos then the sequence of Markov transition kernels $\{K_n\}$ propagates classical molecular chaos.

3.4 Periodic measurement of complete observables

The periodic measurement of a complete observable of a quantum system produces a Markov chain of measurement values.

Let \mathcal{O} be a complete observable of a system, represented by a resolution of the identity $\{|e_j\rangle\langle e_j|\}_{j \in J}$ for some orthonormal basis $\{e_j\}_{j \in J}$ of \mathbb{H} . Consider a (possibly open) quantum system whose evolution is governed by a QDS $(\phi)_t$. If the natural quantum evolution of this system is interrupted periodically by the measurement of \mathcal{O} , then the resulting random sequence of measurement values is a Markov chain on J . To be specific, suppose the measurements of \mathcal{O} are performed at times $0, T, 2T, 3T, \dots$ but there is no other interference with the evolution $(\phi)_t$. The first measurement of \mathcal{O} results in a random outcome, namely, the pure state

$$P_{e_j} = |e_j\rangle\langle e_j|$$

into which the system has collapsed. (We use Dirac notation $|e\rangle\langle e|$ for projection onto the span of e .) In effect, measuring the observable \mathcal{O} prepares a pure state P_{e_j} and informs us of the index $j \in J$ of that pure state. Having been prepared in the state P_{e_j} , the system is allowed to evolve T time units under $(\phi)_t$. By time T , the state of the system is $\phi_{T*}(P_{e_j})$. When \mathcal{O} is measured at time T , the measurement produces another random $j' \in J$, and the system collapses into the corresponding pure state $P_{e_{j'}}$. The probability of the transition $j \rightarrow j'$ is

$$\text{Tr}(\phi_{T*}(P_{e_j})P_{e_{j'}}) = \text{Tr}(P_{e_{j'}}\phi_T(P_{e_j})) \equiv K(j, j'),$$

defining a Markov transition $K(\cdot, \cdot)$ from J to itself. At time T the system has been prepared in some pure state $P_{e_{j'}}$, and a new experiment begins: the system undergoes T time units of the evolution $(\phi)_t$, transforming its state from $P_{e_{j'}}$ to $\phi_{T*}(P_{e_{j'}})$, and then \mathcal{O} is measured at time $2T$, instantaneously forcing the system into the random state indexed by j'' with probability $K(j', j'')$. This is repeated, producing a random record of the indices j_0, j_1, j_2, \dots of the pure states the system was in upon measurement at times $0, 1, 2, \dots$ of \mathcal{O} . Ideally, these successive measurement/experiments would be independent, both physically and stochastically, and it is evident that the performance of those measurements in succession would produce a random sequence j_0, j_1, j_2, \dots governed by the (one-step) Markov transition kernel $K(\cdot, \cdot)$.

It will be convenient to denote by $K[(\phi)_t, \mathcal{O}, T]$ the Markov transition produced in this way, so that

$$K[(\phi)_t, \mathcal{O}, T](j, j') = \text{Tr}(P_{e_j} \phi_T(P_{e_{j'}})). \quad (15)$$

Imagine an n -component system whose (distinguishable) components are each quantum systems with the (same) Hilbert space \mathbb{H} , and which is governed by a QDS $(\phi_n)_t$ that satisfies the permutation condition (6). Let $\{e_j\}$ be an orthonormal basis for \mathbb{H} indexed by J , and let \mathcal{O} be the observable that returns the value j if the (component) system is in the pure state e_j . The observable \mathcal{O} determines a resolution of the identity $\{|e_j\rangle\langle e_j|\}$. The Hilbert space for the n -component system is $\mathbb{H}^{\otimes n}$ and the state of the system is a density operator on $\mathbb{H}^{\otimes n}$. Let \mathcal{O}_i denote the observable that returns the value j if the i^{th} component in the pure state e_j . We can imagine measuring \mathcal{O}_i of each of the components because the components are distinguishable. Simultaneous measurement of $\mathcal{O}_1, \dots, \mathcal{O}_n$ on the n -component system results in a random vector $(j'_1, \dots, j'_n) \in J^n$ of measurement values, and forces the system into the pure state $e_{j'_1} \otimes \dots \otimes e_{j'_n}$. Let \mathcal{O}^n denote the joint measurement $(\mathcal{O}_1, \dots, \mathcal{O}_n)$. Periodic measurement of \mathcal{O}^n results in a Markov chain of values in J^n , since \mathcal{O}^n is a complete observable of the n -component system. The one-step transition kernel for this Markov chain is

$$K[(\phi_n)_t, \mathcal{O}^n, T](\mathbf{j}, \mathbf{j}') = \text{Tr}(P_{e_{j'_1} \otimes \dots \otimes e_{j'_n}} \phi_T(P_{e_{j_1} \otimes \dots \otimes e_{j_n}})). \quad (16)$$

by formula (15).

Corollary 3.7. *Let $(\phi_n)_t$ and \mathcal{O}^n be as above for each n , and suppose that $\{(\phi_n)_t\}$ propagates quantum molecular chaos. Then, for each $T \geq 0$, the sequence of Markov transitions $\{K[(\phi_n)_t, \mathcal{O}^n, T]\}_{n \in \mathbb{N}}$ propagates chaos in the classical sense.*

Proof. Consider the special case of Proposition 3.6 where

$$D(j) = X(j) = |e_j\rangle\langle e_j|.$$

In that case the sequence $\{L_n\}$ of Markov transitions

$$L_n((j_1, \dots, j_n), (j'_1, \dots, j'_n)) = \text{Tr}[(Q_{j_1, \dots, j_n}) \phi_n(Q_{j'_1, \dots, j'_n})] \quad (17)$$

with $Q_{j_1, \dots, j_n} = |e_{j_1}\rangle\langle e_{j_1}| \otimes \cdots \otimes |e_{j_n}\rangle\langle e_{j_n}|$ propagates molecular chaos. But comparing (17) to (16) and noting that

$$\begin{aligned} P_{e_{j_1} \otimes \cdots \otimes e_{j_n}} &= |e_{j_1} \otimes \cdots \otimes e_{j_n}\rangle\langle e_{j_1} \otimes \cdots \otimes e_{j_n}| \\ &= |e_{j_1}\rangle\langle e_{j_1}| \otimes |e_{j_2}\rangle\langle e_{j_2}| \cdots \otimes |e_{j_n}\rangle\langle e_{j_n}| = Q_{j_1, \dots, j_n} \end{aligned}$$

shows that

$$L_n = K[(\phi_n)_t, \mathcal{O}^n, T].$$

□

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