Canonical Emergence of the Density Operator from Normalized Probabilistic Structure

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Abstract

We present a minimal, representation-invariant route from normalized probabilistic structure to operator state description. Starting from probability assignments to admissible effects, we show how simplex-type (context-fixed) descriptions embed into the convex set of density operators as the minimal basis-invariant closure. The key representation is the trace pairing $p(E) = \mathrm{Tr}(\rho E)$, where $\rho \succeq 0$ and $\mathrm{Tr}\rho = 1$. We also formalize composition and marginalization: correlations are encoded by joint states ρ_{AB}, while locally accessible statistics are represented uniquely by reduced states $\rho_A = \mathrm{Tr}_B(\rho_{AB})$. The paper is intentionally conservative: it establishes a logically closed front-end for later developments (modular generators, CPTP-compatible dynamics, and phase structure) without introducing them here as axioms.

1 Introduction: why states must be representation-invariant

Classical probability theory describes a preparation by a point in a simplex: a list of probabilities assigned to mutually exclusive outcomes in a fixed context. In physical practice, however, one must account for changes of representation (e.g., changes of measurement basis or experimental context) without changing the underlying preparation. This motivates the search for a state object that supports a *representation-invariant* probabilistic description.

The density operator ρ is the standard object used in quantum theory for this purpose. The goal of the present paper is not to assume ρ as an axiom, but to isolate a minimal route by which ρ emerges as the canonical, basis-invariant closure of a normalized probabilistic structure. We emphasize (i) convexity and affine structure, (ii) invariance under changes of representation, and (iii) composition and marginalization via partial trace.

Scope. This paper establishes the state-level representation. It does *not* introduce modular generators, modular flow, CPTP dynamics, phase functionals, emergent geometry, or large-N statements beyond a brief outlook; those belong to subsequent papers in the program.

2 Pre-quantum / pre-algebraic layer

This section records a minimal pre-algebraic motivation layer. The technical results of the paper begin in Section 3.

2.1 Pre-state and pre-algebra principles

Axiom 1 (Pre-State Principle)**.** There exists a primitive informational pre-state ω defined on a pre-algebra $\mathcal{A}_0$, encoding the most fundamental relational content prior to any operator-algebraic description.

Axiom 2 (Pre-Algebra Principle)**.** The pre-algebra $\mathcal{A}_0$ is equipped with a primitive relational operation $\star$. Under coarse-graining, this relational structure induces an emergent associative operator-algebraic description.

Definition 1 (Canonical collapse)**.** The canonical collapse is a map

$$\mathcal{C}: \ (\mathcal{A}_0, \omega) \longmapsto (\mathcal{A}, \rho),$$

where $\mathcal{A}$ is an operator algebra encoding coarse-grained observables, and ρ is a normal state on $\mathcal{A}$ representing the induced probabilistic predictions.

Remark 1. Operationally, $\mathcal{C}$ is intended to express a closure principle: a representation-invariant probabilistic description, once required to be stable under admissible changes of representation, forces an operator-state description. The subsequent sections formalize this closure starting from normalized probabilistic structures.

3 Normalized probabilistic structure and the canonical operator realization

3.1 Effects and probability assignments

Let $\mathcal{H}$ be a finite-dimensional Hilbert space. Denote by $B(\mathcal{H})$ the algebra of linear operators on $\mathcal{H}$. An *effect* is an operator $E \in B(\mathcal{H})$ satisfying $0 \preceq E \preceq \mathbb{1}$. A set $\{E_k\}_k$ with $\sum_k E_k = \mathbb{1}$ is a POVM.

Definition 2 (Normalized probabilistic structure)**.** A normalized probabilistic structure is a map

$$p: \ \mathcal{E} \to [0,1], \qquad E \mapsto p(E),$$

defined on a chosen admissible set of effects $\mathcal{E}$, such that:

1. (Normalization) $p(\mathbb{1}) = 1$.
2. (Affineness / convexity) For $E, F \in \mathcal{E}$ and $\lambda \in [0,1]$ with $\lambda E + (1-\lambda)F \in \mathcal{E}$,

$$p(\lambda E + (1-\lambda)F) = \lambda p(E) + (1-\lambda)p(F).$$

This definition captures the empirical requirement that mixing experimental procedures mixes outcome probabilities affinely.

3.2 From simplex states to diagonal density operators

In a fixed context where the admissible effects are diagonal in a chosen orthonormal basis $\{|i\rangle\}_{i=1}^d$, a probabilistic structure corresponds to a probability vector $(p_1, \ldots, p_d)$ and can be represented by the diagonal operator

$$\rho_{\text{diag}} = \sum_{i=1}^{d} p_i \, |i\rangle\langle i|, \qquad p_i \geq 0, \ \sum_i p_i = 1.$$

This is the standard simplex embedding into operators.

3.3 Why basis invariance forces full density operators

The next step is the representation-invariance requirement: descriptions should not depend on the choice of basis. Operationally, a change of representation is modeled by a unitary U acting by conjugation on effects, $E \mapsto UEU^\dagger$. A context-dependent diagonal description is not stable under such changes, which motivates the following elementary closure statement.

Proposition 1 (Diagonal simplex is not closed under basis change)**.** *Let $\mathcal{D} \subset B(\mathcal{H})$ be the set of density operators that are diagonal in a fixed orthonormal basis $\{|i\rangle\}_{i=1}^{d}$. If $d \geq 2$, then $\mathcal{D}$ is not invariant under unitary conjugation: there exist a diagonal $\rho \in \mathcal{D}$ and a unitary U such that $U\rho U^\dagger \notin \mathcal{D}$.*

Proof (sketch). Pick a non-degenerate diagonal state $\rho = \sum_{i=1}^{d} p_i |i\rangle\langle i|$ with $p_1 \neq p_2$. Let U be any unitary that mixes $|1\rangle$ and $|2\rangle$ (e.g., a rotation in span$\{|1\rangle, |2\rangle\}$). Then $U\rho U^\dagger$ has non-zero off-diagonal entries in the original basis, hence it is not diagonal and thus not in $\mathcal{D}$. □

Remark 2. Therefore, any basis-invariant state representation extending simplex-type (diagonal) states must go beyond diagonal operators. The minimal convex, basis-invariant closure leads to the full set of positive trace-one operators (density operators).

3.4 Canonical operator realization

Definition 3 (Density operator)**.** A density operator (quantum state) is an operator $\rho \in B(\mathcal{H})$ such that $\rho \succeq 0$ and $\mathrm{Tr}\rho = 1$.

Theorem 1 (Canonical operator realization)**.** *Any normalized probabilistic structure on admissible effects admits a realization by a density operator ρ such that for all admissible effects E,*

$$p(E) = \mathrm{Tr}(\rho E).$$

Proof (sketch). In a fixed diagonal context, the probabilistic structure is represented by ρ_{diag}. Requiring representation invariance under admissible basis changes forces closure under conjugation, and the previous proposition shows diagonal states are not closed. The minimal convex extension is the set of all density operators. The trace pairing $\mathrm{Tr}(\rho E)$ provides an affine and normalized functional on effects and is stable under simultaneous conjugation $(\rho, E) \mapsto (U\rho U^\dagger, UEU^\dagger)$. Hence the probabilistic structure can be represented in the stated form. □

4 Composition, correlations, and marginalization

4.1 Joint states and local access

Let $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$. A joint state is a density operator $\rho_{AB} \succeq 0$ with $\mathrm{Tr}\rho_{AB} = 1$. Local effects on A correspond to operators of the form $E_A \otimes \mathbb{1}_B$.

Theorem 2 (Reduced state and uniqueness)**.** *For any joint state ρ_{AB} there exists a unique density operator ρ_A on $\mathcal{H}_A$ such that for all local effects E_A,*

$$\mathrm{Tr}\big(\rho_{AB}(E_A \otimes \mathbb{1}_B)\big) = \mathrm{Tr}(\rho_A E_A).$$

Moreover, $\rho_A = \mathrm{Tr}_B(\rho_{AB})$.

Proof (sketch). Define the affine functional on local effects by $f(E_A) = \mathrm{Tr}(\rho_{AB}(E_A \otimes \mathbb{1}_B))$. It is positive and normalized, hence representable as $f(E_A) = \mathrm{Tr}(\rho_A E_A)$ for a unique density operator ρ_A on $\mathcal{H}_A$. By the defining property of the partial trace, this ρ_A equals $\mathrm{Tr}_B(\rho_{AB})$. □

Remark 3 (Interpretation)**.** Joint correlations are encoded in ρ_{AB}. The reduced state ρ_A is the canonical operator representative of locally accessible statistics and can be understood as a principled compression of global correlation structure to the chosen access level.

5 Discussion and outlook

The present paper established a state-level canonical representation: normalized probabilistic structures become operator states under convexity and representation invariance. This supplies the front-end for further structure.

Outlook. Once $(\mathcal{A}, \rho)$ is fixed and ρ is faithful, one may define the modular generator $K_\rho = -\log \rho$ and, in the operator-algebraic setting, the associated modular automorphism group as guaranteed by Tomita–Takesaki theory. This provides a natural backbone for introducing modular dynamics and CPTP-compatible open-system evolution (developed in Paper B). Phase functionals, spectral diagnostics, emergent geometry, and large-N behavior are addressed in subsequent papers.

6 Conclusion

Scientific value

This paper isolates a minimal representation-theoretic passage from normalized probabilistic data to operator states. Its central contribution is to treat a normalized probability assignment $p(\cdot)$ as an affine functional on a convex set of admissible effects and to identify the density operator ρ as the canonical convex, basis-invariant representative realizing the trace pairing

$$p(E) = \mathrm{Tr}(\rho E) \qquad \text{for all admissible effects } E.$$

In particular, the work makes explicit how simplex-type descriptions (diagonal states in a fixed basis) embed into the larger convex state space of positive trace-one operators, and provides a compact closure argument: the diagonal simplex is not invariant under unitary conjugation, hence any basis-invariant extension must pass to the full convex set of density operators.

A second technical value is the explicit treatment of composition and marginalization at the level of functionals. For bipartite systems, the restriction of the global functional to local effects $E_A \otimes \mathbb{1}_B$ is again affine and normalized, and is represented uniquely by the reduced operator $\rho_A = \mathrm{Tr}_B(\rho_{AB})$. This establishes the partial trace as the canonical projection implementing operational locality within the same convex-analytic framework.

Overall, the paper provides a logically closed, methodologically conservative front-end for subsequent developments in which modular generators and dynamical structures are introduced as additional, testable structure rather than axioms.

Potential practical realizations and applications

The operator-state viewpoint developed here supports a range of concrete scientific and applied directions:

1. **Quantum information protocols.** A clean separation between probabilistic functionals $p(\cdot)$ and operator states ρ streamlines the formulation of POVMs, state discrimination, tomography, and resource measures for mixed states.
2. **Open-system modeling and noise engineering.** Density operators interface naturally with CPTP maps and Lindblad-type generators, enabling systematic modeling of decoherence and control in experimental platforms.
3. **Measurement design and calibration.** The explicit state–effect pairing $p(E) = \mathrm{Tr}(\rho E)$ provides a principled framework for designing measurement procedures (including unsharp measurements) and for validating experimental reconstructions of states.
4. **Reproducible numerical pipelines.** The canonical operator representation offers a standardized data object (ρ) for numerical diagnostics, benchmarking of inference procedures, and data-driven exploration of state-space geometry.
5. **Foundational and relational modeling.** By treating ρ as the minimal basis-invariant closure of probabilistic structure, the work provides a conservative foundation for extensions where modular generators, CPTP-consistent dynamics, and phase structure are introduced as additional, testable layers.

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