Quantum coarse graining, symmetries, and reducibility of dynamics

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The common idea behind complexity reduction in physical systems is separation of information into "physically meaningful" and "safely ignorable." Here we consider a generic notion of such separation—implemented by coarse-graining the state space—and address the question of what information is indeed safely ignorable if we want to reduce the complexity of dynamics. The general condition for reducibility of dynamics under coarse graining will be presented for stochastic and quantum systems. In the process we develop the quantum notion of state-space coarse graining that allows us to marginalize selected degrees of freedom. One of our main findings is that there is a broader class of symmetries, beyond those that are considered by Noether's theorem, that can play a role in the reduction of dynamics. Some examples of quantum coarse grainings and the reduction of dynamics with symmetries will be discussed.

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I. INTRODUCTION

The complexity presented by real physical systems is a fundamental challenge that often resists "brute force" calculations but is occasionally manageable with some analytical insight. The idea of coarse graining (CG) is a prime example of such insight, and its use in physics traces back to the Ehrenfests' work on statistical mechanics [1]. Today, there are many forms in which CG appears in physics: renormalization methods in condensed matter [2,3], coarse-grained modeling of biomolecular dynamics [4], and separation of scales in cosmology [5] are some of the common examples. Nonetheless, there is a common, system-independent notion of CG that underlines all such approaches, and that is the abstract notion of *state-space coarse graining* (from here on by "CG" we will refer to this abstract notion). Studying the implications of such generic notion of CG is therefore essential for our understanding of complexity reduction in physical systems on a fundamental level.

The notion of CG is an elementary proposition in statistical mechanics which asserts that if one is unable to distinguish some states of the system, then the system is described by a smaller (coarser) state space of distinguishable states. In the context of thermodynamics, CG is manifested by our inability to measure microstates of the system, leading to the definition of macrostates described by variables such as temperature and pressure. Another common manifestation of CG is the situation where a composite system has an inaccessible subsystem. Our inability to distinguish between states that differ only by the inaccessible part leads to a coarser description which we account for by marginalizing the inaccessible subsystem.

Despite its origin as a manifestation of practical limitations, the notion of CG is generic, specified only by the choice of indistinguishable states. Therefore, we can consider CG as a generic way to introduce ignorance without relying on any physical structure of the system.

The simple classical notion of CG does not translate naturally into quantum theory and recently there have been multiple proposals for its extension. In Ref. [6], quantum CG was implemented by coarse-graining the quasiprobability (Wigner function) representation of an N-qubit system. The authors of [7] argue that any dimension-reducing quantum channel can be interpreted as a quantum CG. In Ref. [8], CG of the Hilbert space was specified by a set of preferred states and implemented with the statistical method of principal component analysis. Finally, in Ref. [9], the quantum notion of CG was presented as the effective state space perceived by a constrained observer.

The goal of current work is twofold: (a) establish the quantum notion of CG by direct analogy with the classical concept and provide it with operational meaning; (b) develop the framework for complexity reduction of dynamics with CG and integrate it with the framework of symmetries. We will initially work out the main concepts in the more intuitive setting of classical stochastic systems, and then proceed to the finite-dimensional quantum setting. The stochastic case will be accompanied by analysis of out-of-equilibrium dynamics of a 1D Ising chain. In the quantum setting we will discuss some special cases of the CG map and analyze the dynamics of a continuous-time quantum walk on a binary tree.

In order to formulate the quantum notion of CG as closely as possible to the classical case, we will first establish it in the context of stochastic systems. The key observation here is that CG can be interpreted as a marginalization of a kind of subsystem (we will call it a *partial* subsystem and it generalizes the idea of a *virtual* subsystem [10]). This will allow us to formulate the quantum notion of CG by a direct analogy. The result is a dimension-reducing map that implements a quantum CG scheme according to specifications that resemble the classical choice of indistinguishability. Furthermore, the specification of quantum CG will be directly related to a restricted set of observables that give it operational meaning.

The main application we will focus on is reduction of dynamics. The key problem is identifying such CGs that allow

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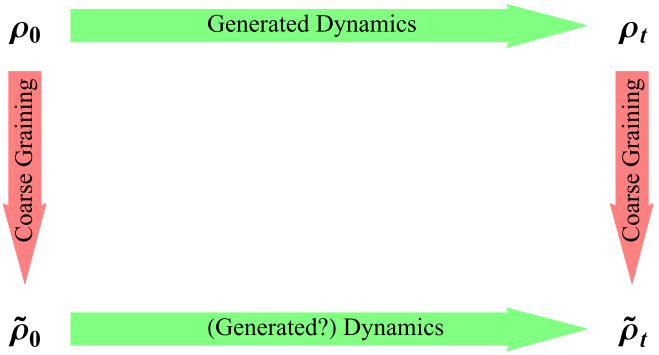


FIG. 1. Dynamics of coarse-grained states cannot be generated unless the coarse-graining scheme is *compatible* with the original generator of dynamics.

time evolutions in the reduced state space to be governed by a reduced generator of dynamics. This can be summarized with the diagram in Fig. 1. In general, time evolutions in the reduced state space are not even uniquely determined by initial conditions, and when they are they may still lose the semigroup structure necessary for the existence of the generator of dynamics [11]. Therefore, it is important to understand the compatibility condition between CG and dynamics that allows the preservation of semigroup structure in the reduced state space. We will provide the general version of such condition in Theorem 1, which applies to both stochastic and quantum systems, and specialize it to unitary dynamics in Theorem 3.

Symmetries turn out to play an important role in the analysis of reducibility of dynamics. We will see that symmetrization of the state space with respect to some group representation is a special case of CG. Inserting this case into the general compatibility conditions between CG and dynamics leads to a broader class of symmetries relevant in the analysis of dynamical evolutions. The new symmetries are defined in Theorems 2 (stochastic) and 4 (quantum) by a compatibility condition with the generator of dynamics. In both stochastic and quantum cases, the compatibility condition extends the relevant symmetries beyond those that commute with time evolutions, as considered by Noether's theorem.

II. CLASSICAL COARSE GRAINING

Before we formally define CG for discrete stochastic systems, it is worth having a concrete, albeit generic, example.

Consider a random walk on the graph of Fig. 2(a). The weights on the edges represent the rate (probability per unit time) of transitions between connected vertices in both directions. Parameters a, b, c, d, e are all positive and the rest obey $|\delta|,|\epsilon| \leqslant \frac{c}{2}$, such that all rates are non-negative. If we coarse-grain this system by choosing not to distinguish between vertices that appear in the same column, then we partition it into 3 blocks associated with the macrostates:

$$u_1 = \{v_1\}, \quad u_2 = \{v_2, v_3\}, \quad u_3 = \{v_4, v_5, v_6\}.$$

The question now is what values can we assign, if any, to the transition rates between the macrostates.

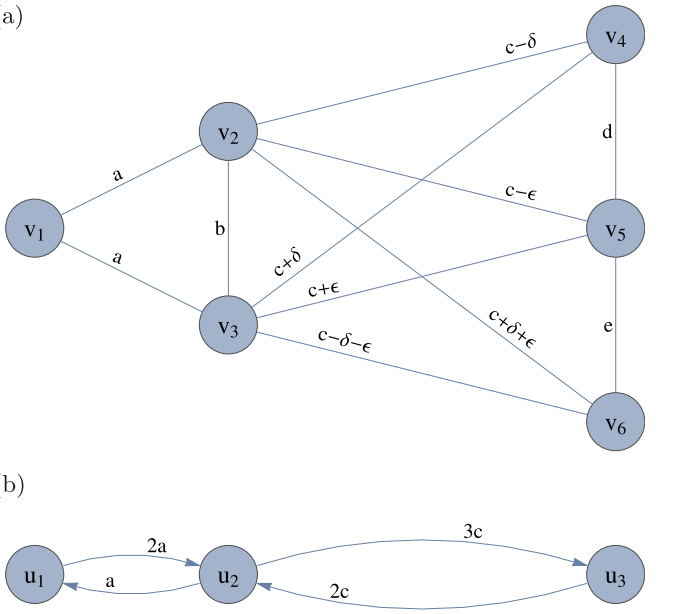


FIG. 2. (a) Random walk graph with transition rates specified on the edges. (b) Coarse-grained graph where the vertices in the same column are blocked together. Effective transition rates between columns are specified on directed edges.

If we consider a single vertex, say v_2, and sum all the transition rates from v_2 to the column on the right, we get

$$\sum_{v \in u_3} r(v_2 \to v) = 3c.$$

We will get the same value if instead of v_2 we take v_3. Therefore, the rate of transitions from *any* vertex in the middle column to the right column is $3c$. This unambiguously defines the rate of transition from the middle column to the right column, without reference to any particular vertex. Similarly, the rate of transitions from any vertex in the right column to the middle column is $2c$. We can repeat this argument for transitions between the left and the middle columns, yielding the rates of $2a$ and a in the opposing directions. We should also note that there are no direct transitions between the leftmost and the rightmost columns. Therefore, transition rates between all three columns are well defined and shown in Fig. 2(b).

The fact that we can get a well-defined random walk in the reduced state space is not trivial. Such reduction of dynamics is only possible when the rate of transitions between the chosen macrostates is unambiguous. Choosing a slightly different CG, where the macrostates are

$$u_1 = \{v_1, v_2, v_3\}, \quad u_2 = \{v_4, v_5, v_6\},$$

results in undefined transition rates. That is because the rate of transitions from v_1 to any vertex in u_2 is 0, but from v_2 or v_3 it is $3c$. Given that the initial macrostate is u_1, it is impossible to tell what the initial rate of transitions to u_2 will be, because it depends on where inside u_1 it actually starts. Similarly, the original choice of CG by the columns would not work if we slightly change the dynamics by altering the transition rate between v_1 and v_2 to $\tilde{a} \neq a$. Now, it is not possible to tell the

rate of transitions from the middle column to the left because it depends on the internal state of the column.

This example demonstrates the fact that it may be possible to generate time evolutions in the coarse-grained state space but the original dynamics and the CG have to be compatible. Such compatibility does not imply that the rates of transition must be uniform; in general all 6 rates between vertices in the middle and the right columns in Fig. 2(a) can be different. We will prove that the necessary and sufficient condition for such compatibility in Markovian stochastic systems is what we already noted: the *total* rate of transitions from *any* state in one block to another should be constant.

A. Formal definition

Classical indistinguishability of states can be specified by an equivalence relation that partitions the state space into equivalence classes of *macro*states. If we consider the system with a discrete and finite state space $\mathsf{A} := \{\alpha_i\}_{i=1}^{|\mathsf{A}|}$, we can specify its CG by the set $\mathsf{B} := \{\beta_k\}_{k=1}^{|\mathsf{B}|}$ of disjoint subsets of A that partition A. If we order the set A consistently with the partition we can identify blocks of indices $b_k := \{i_k, i_k+1, \ldots\}$ such that $\beta_k := \{\alpha_i\}_{i\in b_k}$. The system is said to be in a macrostate β_k if it is in *any* of the microstates $\alpha_i \in \beta_k$.

Probabilistic microstates (macrostates) of the system live in the vector space $\mathbb{R}^{\mathsf{A}}$ ($\mathbb{R}^{\mathsf{B}}$) of real-valued functions p from A (B) to $\mathbb{R}$ which, if positive and normalized, are interpreted as probability distributions over the states A (B). By definition of the macrostates, the probability of finding the system in a macrostate β is the probability of finding it in *any* microstate $\alpha \in \beta$, that is,

$$p_{\mathsf{B}}(\beta) = \sum_{\alpha\in\beta} p_{\mathsf{A}}(\alpha). \tag{1}$$

Since $\mathbb{R}^{\mathsf{A}}$ ($\mathbb{R}^{\mathsf{B}}$) is just an $|\mathsf{A}|$ ($|\mathsf{B}|$) dimensional vector space, we can express relation (1) as a vector equation $p_{\mathsf{B}} = M p_{\mathsf{A}}$ and M is a $|\mathsf{B}| \times |\mathsf{A}|$ block diagonal matrix of the form

$$M := \begin{pmatrix} 1 & \cdots & 1 & & & \\ & & & \ddots & & \\ & & & & 1 & \cdots & 1 \end{pmatrix}, \tag{2}$$

where the kth block is a $1 \times |\beta_k|$ row-vector filled with 1's. M acts by summing the fine-grained probability distribution in each block of microstates into a single value, which is the total probability of finding the system in *any* microstate of that block. We will call such M a *coarse-graining matrix*.

Any CG matrix M admits the right inverse M^+ such that $MM^+ = I$ is an identity on $\mathbb{R}^{\mathsf{B}}$. It is easy to check that it is the $|\mathsf{A}| \times |\mathsf{B}|$ block diagonal matrix of the form

$$M^+ := \begin{pmatrix} |\beta_1|^{-1} & & & & \\ \vdots & & & & \\ |\beta_1|^{-1} & & & & \\ & \ddots & & & \\ & & & |\beta_{|\mathsf{B}|}|^{-1} & \\ & & & \vdots & \\ & & & |\beta_{|\mathsf{B}|}|^{-1} \end{pmatrix}, \tag{3}$$

where the kth block is a $|\beta_k| \times 1$ column-vector filled with $|\beta_k|^{-1}$. This is the Moore-Penrose pseudoinverse [12] of M, which means that $P := M^+M$ is an orthogonal projection on the subspace $(\ker M)^\perp \subseteq \mathbb{R}^{\mathsf{A}}$. Moreover, restriction of M to $(\ker M)^\perp$ is an isomorphism $M : (\ker M)^\perp \longrightarrow \operatorname{im} M$ and since $(\ker M)^\perp = \operatorname{im} P$ and $\operatorname{im} M = \mathbb{R}^{\mathsf{B}}$ it follows that $\operatorname{im} P \cong \mathbb{R}^{\mathsf{B}}$. The isomorphism between the image of P and the image of M implies that P erases the same fine-grained information as M. We will call P a *coarse-graining projection* which has the block diagonal form

$$P := \begin{pmatrix} |\beta_1|^{-1} & \ldots & |\beta_1|^{-1} & & & & \\ \vdots & \ddots & \vdots & & & & \\ |\beta_1|^{-1} & \ldots & |\beta_1|^{-1} & & & & \\ & & & \ddots & & & \\ & & & & |\beta_{|\mathsf{B}|}|^{-1} & \ldots & |\beta_{|\mathsf{B}|}|^{-1} \\ & & & & \vdots & \ddots & \vdots \\ & & & & |\beta_{|\mathsf{B}|}|^{-1} & \ldots & |\beta_{|\mathsf{B}|}|^{-1} \end{pmatrix}, \tag{4}$$

where the kth block is a $|\beta_k| \times |\beta_k|$ matrix filled with $|\beta_k|^{-1}$. P acts by averaging over the probabilities in each block. The advantage of P over M is that P leaves the result of CG in the subspace of $\mathbb{R}^{\mathsf{A}}$, which allows a direct comparison of states before and after CG.

B. Compatibility with dynamics

In this section we show how this notion of CG allows us to study the dynamics of some select properties of the system without the need to understand the dynamics of all its degrees of freedom. We will focus on continuous-time Markov processes (CTMPs) because they are common in classical models and are closely related to quantum dynamics.

The idea is that given a dynamical system we can coarse-grain it and derive dynamical rules that generate consistent time evolutions in the coarse-grained state space (see Fig. 1). We will say that CG is *compatible* with dynamics if there is a generator that governs time evolutions in the reduced state space. The main question that we address here is how to recognize compatible CGs and how to derive the reduced generator.

The dynamical rules of CTMPs can be specified with a *transition rate matrix* Q such that [13]

$$\frac{d}{dt} p_{\mathsf{A}} = Q\, p_{\mathsf{A}} \tag{5}$$

for $p_{\mathsf{A}} \in \mathbb{R}^{\mathsf{A}}$. The off-diagonal elements Q_{ij} specify the rate of transitions between states $\alpha_j \longmapsto \alpha_i$ while the diagonal elements $Q_{jj} := -\sum_{i\neq j} Q_{ij}$ specify the total rate of transitions out of states α_j. For an initial probabilistic state $p_{\mathsf{A}}(0)$, the subsequent states are given by the solutions of Eq. (5) as $p_{\mathsf{A}}(t) = e^{tQ} p_{\mathsf{A}}(0)$, where Q generates time evolutions similarly to the Hamiltonian in quantum mechanics (strictly speaking Q is closer in nature to the Lindblad operator rather than the Hamiltonian).

Now, consider a CG B of A represented by the matrix $M : \mathbb{R}^{\mathsf{A}} \longrightarrow \mathbb{R}^{\mathsf{B}}$. The coarse-grained probabilistic state evolves

according to $p_{\mathsf{B}}(t) := M p_{\mathsf{A}}(t)$ and *a priori* there is no reason to assume that it also evolves as a CTMP. However, this is exactly what we require from the compatibility of CG with dynamics in order to be able to generate time evolutions in the reduced state space. The following theorem provides the necessary and sufficient conditions for it to be true.

Theorem 1. Let Q be a transition rate matrix as in Eq. (5), let M be a coarse-graining matrix as in Eq. (2), and let P be a coarse-graining projection as in Eq. (4). Then, the coarse-grained state $p_{\mathsf{B}} := M p_{\mathsf{A}}$ evolves as a CTMP for all p_{A} if and only if

$$PQ = PQP. \tag{6}$$

The reduced transition rate matrix $\tilde{Q}$ such that $\frac{d}{dt} p_{\mathsf{B}} = \tilde{Q}\, p_{\mathsf{B}}$ is then given by $\tilde{Q} := MQM^{+}$.

Proof. If $PQ = PQP$ then multiplying it by M on the left we get $MQ = MQM^{+}M$ and therefore

$$\frac{d}{dt} p_{\mathsf{B}} = M \frac{d}{dt} p_{\mathsf{A}} = MQ p_{\mathsf{A}} = \tilde{Q} p_{\mathsf{B}},$$

where $\tilde{Q} = MQM^{+}$. This proves the "if" direction.

On the other hand if p_{B} evolves as a CTMP then there is a $\tilde{Q}$ such that $\frac{d}{dt} p_{\mathsf{B}} = \tilde{Q}\, p_{\mathsf{B}}$. Therefore

$$MQ p_{\mathsf{A}} = M \frac{d}{dt} p_{\mathsf{A}} = \frac{d}{dt} p_{\mathsf{B}} = \tilde{Q}\, p_{\mathsf{B}} = \tilde{Q} M p_{\mathsf{A}}.$$

Since it has to hold for all p_{A} we are left with $MQ = \tilde{Q}M$. Multiplying it by M^{+} from the right we get $\tilde{Q} = MQM^{+}$. If we substitute $\tilde{Q}$ back into $MQ = \tilde{Q}M$ and multiply by M^{+} from the left we get $PQ = PQP$. Hence the "only if." ■

Thus, for example, in the case of random walk of Fig. 2(a) with CG by the columns, we have the CG matrix

$$M := \begin{pmatrix} 1 & & & & & \\ & 1 & 1 & & & \\ & & & 1 & 1 & 1 \end{pmatrix},$$

$$M^{+} := \begin{pmatrix} 1 & & \\ & 1/2 & \\ & 1/2 & \\ & & 1/3 \\ & & 1/3 \\ & & 1/3 \end{pmatrix},$$

and the transition rate matrix (diagonal elements are just the negatives of the column's sum)

$$Q := \begin{pmatrix} Q_{11} & a & a & 0 & 0 & 0 \\ a & Q_{22} & b & c-\delta & c-\epsilon & c+\delta+\epsilon \\ a & b & Q_{33} & c+\delta & c+\epsilon & c-\delta-\epsilon \\ 0 & c-\delta & c+\delta & Q_{44} & d & 0 \\ 0 & c-\epsilon & c+\epsilon & d & Q_{55} & e \\ 0 & c+\delta+\epsilon & c-\delta-\epsilon & 0 & e & Q_{66} \end{pmatrix}.$$

It is straightforward to check that the compatibility condition (6) holds and the reduced transition rate matrix is

$$\tilde{Q} = MQM^{+} = \begin{pmatrix} -2a & a & 0 \\ 2a & -3c-a & 2c \\ 0 & 3c & -2c \end{pmatrix}.$$

This matrix generates the random walk of Fig. 2(b).

The compatibility condition (6) has an intuitive interpretation. If we understand the image of P to be the subspace of coarse-grained states, then the image of $P^{\perp} := I - P$ must be the subspace containing fine-grained information. The compatibility condition $PQ = PQP$ is equivalent to $PQP^{\perp} = 0$ which means that Q does not map fine-grained information into the coarse-grained subspace. Then, time evolution of the coarse-grained state cannot be affected by the fine-grained details. This is a sensible requirement because if fine-grained details could affect coarse-grained evolution, it would not be possible to throw them away and expect to tell how the coarse-grained state will evolve.

In more concrete terms, what the compatibility condition ensures is that the rate of transitions between macrostates is a well-defined property. To see that, let us try to derive the rate of transition between macrostates from the original rates between microstates. The total rate of transitions from a microstate $\alpha_i \in \beta_k$ to any microstate in $\beta_{k'}$ $(k \neq k')$ is given by $r(\alpha_i \longmapsto \beta_{k'}) := \sum_{j \in b_{k'}} Q_{ji}$. If the value of $r(\alpha_i \longmapsto \beta_{k'})$ varies with different $\alpha_i \in \beta_k$ then knowledge of the initial macrostate β_k is not enough to tell the rate of transitions to $\beta_{k'}$. But if $r(\alpha_i \longmapsto \beta_{k'})$ is the same for all $\alpha_i \in \beta_k$ then it does not matter in which microstate of β_k we start; the rate of transitions from β_k to $\beta_{k'}$ is given by $r(\alpha_i \longmapsto \beta_{k'})$ for any $\alpha_i \in \beta_k$. Therefore, the notion of rate of transitions between macrostates is meaningless unless the rates $r(\alpha_i \longmapsto \beta_{k'})$ are uniform over $\alpha_i \in \beta_k$ for all β_k and $\beta_{k'}$. The following corollary to Theorem 1 formalizes this argument.

Corollary 1. Let Q be a transition rate matrix and

$$r(\alpha_i \longmapsto \beta_{k'}) := \sum_{j \in b_{k'}} Q_{ji}$$

the total rate of transitions from $\alpha_i \in \beta_k$ to $\beta_{k'}$. Then the compatibility condition $PQ = PQP$ is equivalent to $r(\alpha_i \longmapsto \beta_{k'})$ being constant over the subset β_k, for all β_k and $\beta_{k'}$.

Proof. By definition of P [Eq. (4)] we calculate the matrix elements of PQ to be

$$(PQ)_{i'i} = \sum_{j=1}^{|\mathsf{A}|} P_{i'j} Q_{ji} = \frac{1}{|\beta_{k'}|} \sum_{j \in b_{k'}} Q_{ji} = \frac{r(\alpha_i \longmapsto \beta_{k'})}{|\beta_{k'}|},$$

where k' is the index of the block such that $i' \in b_{k'}$. Similarly the matrix elements of PQP are

$$(PQP)_{i'i} = \sum_{j=1}^{|\mathsf{A}|} (PQ)_{i'j} P_{ji} = \frac{1}{|\beta_k|} \sum_{j \in b_k} (PQ)_{i'j}$$
$$= \frac{1}{|\beta_k||\beta_{k'}|} \sum_{j \in b_k} r(\alpha_j \longmapsto \beta_{k'}),$$

where k is the index of the block such that $i \in b_k$. Elementwise, the condition $PQ = PQP$ then reads

$$r(\alpha_i \longmapsto \beta_{k'}) = \frac{1}{|\beta_k|} \sum_{j \in b_k} r(\alpha_j \longmapsto \beta_{k'}).$$

The right-hand side depends on i only through the block index k; therefore this condition states that $r(\alpha_i \longmapsto \beta_{k'})$ is constant for all $\alpha_i \in \beta_k$.

On the other hand if $r(\alpha_i \longmapsto \beta_{k'})$ is constant for all $\alpha_i \in \beta_k$, then

$$(PQP)_{i'i} = \frac{1}{|\beta_k||\beta_{k'}|} \sum_{j \in b_k} r(\alpha_j \longmapsto \beta_{k'})$$
$$= \frac{1}{|\beta_{k'}|} r(\alpha_i \longmapsto \beta_{k'}) = (PQ)_{i'i}.$$

■

It is worth pointing out the compatibility condition of Corollary 1 is the defining property of an *equitable partition* of a weighted graph specified by Q [14]. The problem of finding a CG compatible with dynamics is therefore equivalent to the problem of finding an equitable partition of the weighted graph specified by Q.

C. Coarse graining and symmetries

So far we have specified CG with the choice of equivalence classes that determine indistinguishable states. In the following we show how CG can also be specified with group representations.

Proposition 1. Let G be a group that permutes elements of the state space A, and let the permutation matrices $D(G)$ be its representation on $\mathbb{R}^{\mathsf{A}}$. Then, the symmetrizer $P := |G|^{-1} \sum_{g \in G} D(g)$ is a coarse-graining projection associated with partition of A into orbits of G.

Proof. To show that P is a CG projection for any G it is sufficient to show that it acts as a CG projection on any basis element $\hat{\alpha} \in \mathbb{R}^{\mathsf{A}}$ (for clarity we omit the element's index). For a given $\hat{\alpha}$ we define the subgroup that stabilizes it as $G_\alpha := \{g \in G \mid g(\alpha) = \alpha\}$. Since cosets of G_α form a partition of G we can write

$$P = |G|^{-1} \sum_{C \in G/G_a} \sum_{g \in C} D(g),$$

where C runs over all distinct cosets. If $g_1, g_2 \in C$ belong to the same coset of G_α then clearly $g_1(\alpha) = g_2(\alpha)$. On the other hand if g_1, g_2 belong to different cosets then $g_1(\alpha) = g_2(\alpha)$ implies $g_1^{-1} g_2 \in G_\alpha$ so $g_2 = g_1 h$ for some $h \in G_\alpha$ but that contradicts their residence in different cosets; therefore $g_1(\alpha) \neq g_2(\alpha)$. Applying these rules and denoting with $G(\alpha)$ the orbit of α, we get

$$P\hat{\alpha} = |G|^{-1} \sum_{C \in G/G_a} \sum_{g \in C} D(g)\hat{\alpha}$$
$$= |G_a|/|G| \sum_{C \in G/G_a} D(g \in C)\hat{\alpha}$$
$$= |G_a|/|G| \sum_{\alpha' \in G(\alpha)} \hat{\alpha}'.$$

It is a well-known consequence of the orbit-stabilizer theorem [15] that $|G|/|G_a| = |G(\alpha)|$, so in fact

$$P\hat{\alpha} = |G(\alpha)|^{-1} \sum_{\alpha' \in G(\alpha)} \hat{\alpha}'.$$

Recalling the general form of a CG projection (4), we see that P acts on $\hat{\alpha}$ as the CG projection constructed from partition of A into orbits of G. ■

Thus, any group G acting on A specifies a CG associated with the orbits of G. Then, if we treat symmetrizations as a special case of CG, we can specialize the general compatibility condition of Theorem 1 to this case and express it in terms of group representations.

Theorem 2. Let

$$P = |G|^{-1} \sum_{g \in G} D(g) \tag{7}$$

be a symmetrizer with respect to a group G, and let Q be a transition rate matrix. Then, the compatibility condition $PQ = PQP$ is equivalent to

$$P \sum_{g \in G} [D(g), Q] = 0. \tag{8}$$

If in addition $Q = Q^T$, then it simplifies to

$$\sum_{g \in G} [D(g), Q] = 0. \tag{9}$$

Proof. By definition (7) of P and the fact that $P = P^2$ we get

$$PQP = |G|^{-2} \sum_{g,g' \in G} D(g) Q D(g')$$
$$= |G|^{-2} \sum_{g,g' \in G} D(g)(D(g')Q - [D(g'), Q])$$
$$= \left(|G|^{-1} \sum_{g \in G} D(g) \right) \left(|G|^{-1} \sum_{g' \in G} D(g') \right) Q$$
$$- |G|^{-1} \left(|G|^{-1} \sum_{g \in G} D(g) \right) \left(\sum_{g' \in G} [D(g'), Q] \right)$$
$$= PQ - |G|^{-1} P \left(\sum_{g' \in G} [D(g'), Q] \right),$$

hence the equivalence to (8). If in addition $Q = Q^T$, then $PQ = PQP$ implies

$$QP = (PQ)^T = (PQP)^T = PQP = PQ,$$

that is $[P,Q]=0$. And also $[P,Q]=0$ implies $PQ=PQP$ hence the equivalence to (9). ■

As was pointed out after Corollary 1, CGs that are compatible with dynamics form an equitable partition of the graph specified by the weighted adjacency matrix Q. In Ref. [14], graph automorphism symmetries (permutations of vertices that commute with the weighted adjacency matrix Q) were used to single out equitable partitions with their orbits. Theorem 2 confirms this, as Eq. (8) trivially holds for all groups that satisfy $[D(g),Q]=0$ for all g. However, Theorem 2 (together with Corollary 1) implies that there is a broader set of symmetries, beyond automorphisms, that specify equitable partitions with their orbits. These are the groups that comply with Eq. (8) or (9).

D. Example: Glauber-Ising model

The system that we study here is a 1D classical spin lattice with periodic boundary conditions, i.e., an Ising spin chain. We will see that compatible CGs of this system are not so obvious (and the obvious ones are not compatible). We will overcome this difficulty by putting to use the considerations of symmetry developed in the previous section.

Each of the sites in the Ising chain can be in one of two states $\{\pm1\}$. A microstate of the lattice of length N is an N-component binary vector $\sigma\in\{\pm1\}^N$, and the state space consists of 2^N microstates $\{\sigma_i\}_{i=1}^{2^N}$. The internal energy of a microstate σ is

$$E(\sigma)=-J\sum_{x=1}^{N}\sigma^{(x)}\sigma^{(x+1)},$$

where $J>0$ is the local interaction energy, and $\sigma^{(x)}$ is the sign of site x.

The Glauber-Ising model, proposed by Glauber in Ref. [16], is a model of dynamics for an Ising spin chain that interacts thermally with its environment. According to the model, the microstate of the system evolves by transitions caused by single spin flips. The transition rate depends on whether the energy increases, decreases, or stays the same:

$$r(\sigma\longmapsto\sigma'):=\begin{cases}1-\gamma(T) & :\ E(\sigma')>E(\sigma),\\ 1 & :\ E(\sigma')=E(\sigma),\\ 1+\gamma(T) & :\ E(\sigma')<E(\sigma),\end{cases}$$

where $\gamma(T)$ is a positive, temperature-dependent parameter. This model simply states that transitions that increase E happen at a slower rate than the ones that decrease E, and this rate difference is additively modified by the temperature through $\gamma(T)$. All three rates are in units that normalize the middle rate to 1. The parameter $\gamma(T)$ can then be derived by demanding detailed balance condition in equilibrium, which leads to $\gamma(T)=\tanh\left[\frac{2J}{T}\right]$ (see [16] for details). With the rate function $r(\sigma\longmapsto\sigma')$ we can in principle construct the $2^N\times2^N$ transition rate matrix Q.

In order to understand how this dynamical system can be coarse-grained, we look at the case of $N=3$ first. Instead of writing down the matrix Q explicitly, we describe the dynamics as a random walk on the graph depicted in Fig. 3(a). The signs $\pm$ stand for ±1 and transition rates are explicitly specified only where they differ from 1. The total transition rate from each of the ground states $(+++)$, $(---)$, to the bulk of excited states (the ones in the middle) sum to $3(1-\gamma)$. In the opposite direction, from excited to the ground, there is only one transition for each of the excited states, and it is at the same rate $1+\gamma$. Corollary 1 then implies that coarse graining this system with respect to the energy levels is compatible with dynamics. Instead of energy we can count the number of domains d (defined as half the number of intervals in the chain that differ in sign from their surroundings) which is a proxy variable for energy as seen from the relation $E=-J(N-4d)$. In Fig. 3(b) we see the reduced state space, coarse-grained by blocking together microstates that have the same energy or number of domains.

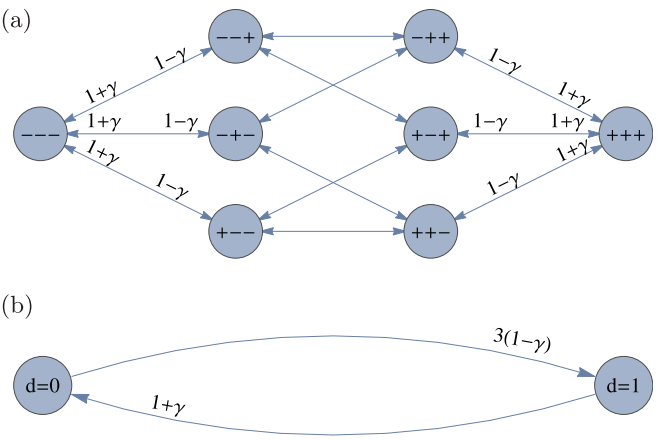


FIG. 3. (a) Random walk graph for a 3-spin Ising chain. Glauber's transition rates are explicitly specified on the edges only where they differ from 1. Transition rate 1 is implied for unlabeled edges. (b) Coarse graining of the state space of 3-spin Ising chain with respect to the total number of domains d. Effective transition rates between states with $d=0$ and $d=1$ specified on the edges.

The reduced transition rate matrix

$$\tilde{Q}=\begin{pmatrix}-3(1-\gamma) & 1+\gamma\\ 3(1-\gamma) & -1-\gamma\end{pmatrix}$$

generates a random walk in the state space of the number-of-domains variable $d\in\{0,1\}$. The eigenvalues of $\tilde{Q}$ are $\lambda_0=0$ and $\lambda_1=2(\gamma-2)$ which correspond to the eigenvectors

$$v_0=\frac{1}{2(2-\gamma)}\begin{pmatrix}1+\gamma\\ 3(1-\gamma)\end{pmatrix},\quad v_1=\begin{pmatrix}-1/2\\ 1/2\end{pmatrix}.$$

Since $e^{t\tilde{Q}}v_0=v_0$, the vector v_0 is the steady or equilibrium state of the system, and its components are the probabilities of finding the system in one of the energy levels when the system is in equilibrium. So, for example, the probability of finding this system in the excited state in equilibrium is

$$\Pr(E=J)=\frac{3\left(1-\tanh\left[\frac{2J}{T}\right]\right)}{2\left(2-\tanh\left[\frac{2J}{T}\right]\right)}=\frac{3}{3+e^{4J/T}}.$$

This expression agrees with the standard calculation of Boltzmann's factor and partition function.

In addition to recovering equilibrium properties from $\tilde{Q}$, we can also learn something about out-of-equilibrium behavior. Since v_0 is a normalized probability vector, we can always add to it a fraction of v_1 to get any other normalized probability

vector. So, any initial state p_{in} can be written as $v_0 + r v_1$, where r is a real parameter. Its time evolution is then given by

$$p(t) = e^{t\tilde{Q}} p_{in} = v_0 + r e^{t\lambda_1} v_1.$$

Note that $\lambda_1 < -2$ because $\gamma = \tanh[\frac{2J}{T}] < 1$; therefore every initial state relaxes to equilibrium v_0 by exponentially suppressing v_1. This means that the characteristic relaxation time for this system is

$$-\frac{1}{\lambda_1} = -\frac{1}{2(\gamma - 2)} = \frac{1}{2}\left(\frac{1 + e^{4J/T}}{3 + e^{4J/T}}\right).$$

Even though the intuitive CG with respect to the energy levels is compatible with dynamics for $N = 3$, it is not true in general (see the case of $N = 4$ below). In the general case we will look for a group that complies with the compatibility condition of Theorem 2, and take its orbits to be the compatible CG blocks.

From the $N = 3$ case we see that the group $\mathbb{Z}_3$ of lattice translations generates orbits that coincide with columns in Fig. 3(a). If we complement this group with $\mathbb{Z}_2$ of global spin flips then $\mathbb{Z}_3 \times \mathbb{Z}_2$ generates 2 orbits that coincide with the blocks of $d = 0$ and $d = 1$. Since these blocks are compatible with dynamics, we conjecture that for general N the orbits of $G = \mathbb{Z}_N \times \mathbb{Z}_2$ (translations and global flips) are compatible with dynamics.

To prove that, we note that the transition rate matrix can be decomposed as a sum of N matrices $Q = \sum_{x=1}^{N} Q^{(x)}$, where each $Q^{(x)}$ generates transitions restricted to flips of site x. If $D(x)$ represents the action of lattice translations by x sites, and $D(x)D(y) = D(x + y)$, then we get

$$D(y)Q^{(x)} = D(y)Q^{(x)}D(-y)D(y) = Q^{(y+x)}D(y).$$

Therefore,

$$D(y)Q = \sum_{x \in \mathbb{Z}_N} Q^{(y+x)}D(y) = QD(y),$$

that is $[D(y), Q] = 0$. Each local spin flip generator $Q^{(x)}$ also commutes with the global spin flip action $D(f)$; therefore $[D(g), Q] = 0$ for all $g \in G$. Since G is a symmetry group of Q, it satisfies the compatibility condition of Theorem 2, and we can coarse-grain this dynamical system by blocking together the states that belong to the same orbit of G.

For $N = 4$ the orbits of G are

$$\begin{aligned}
&d = 0 \quad \{\text{orbit 1} \quad \{(++++) \quad (----),\\
&d = 1 \quad \begin{cases} \text{orbit 2} & \begin{cases} (+--+) & (-++-), \\ (-+-+) & (+-+-), \\ (--++) & (++--), \\ (---+) & (+++-), \end{cases} \\ \text{orbit 3} & \begin{cases} (++--) & (--++), \\ (-++-) & (+--+), \end{cases} \end{cases}\\
&d = 2 \quad \{\text{orbit 4} \quad \{(+-+-) \quad (-+-+),
\end{aligned}$$

so orbit 1 coincides with the lowest energy level, orbits 2 and 3 together form the first excited level, and orbit 4 coincides with the second excited level. Transition rates between the orbits are shown in Fig. 4. Note that the rate of transitions from orbit 2 to

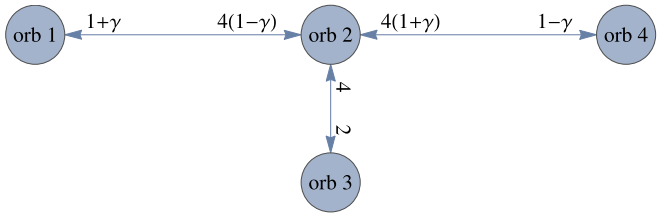


FIG. 4. Random walk graph for a 4-spin state space coarse-grained with respect to orbits of translations and global spin flips.

the neighboring energy levels is $1 \pm \gamma$ but from orbit 3 it is 0, because no single spin flip can change the energy. In general, the total transition rates to the neighboring energy levels are not constant over the states in each energy level. That is why CG by energy levels is not compatible with dynamics. For $N > 3$ energy levels happen to be too coarse to be compatible, but the orbits of G are fine enough.

It is curious to note that in the thermodynamic limit $N \longrightarrow \infty$, each energy level consists almost entirely of states that have the same total transition rate to the neighboring levels. The nonuniformity of rates over the energy levels is then suppressed, and transition rates between energy levels can be approximately defined, but this analysis is beyond our scope here.

E. Partial subsystems and bipartitions

The concept of a partial subsystem that we will define here is a natural by-product of the CG discussion. It follows from the observation that for a bipartite system, marginalization of one of its subsystems is a special case of CG. If so, it is natural to ask whether any CG can be viewed as marginalization of some kind of subsystem. The answer is yes if one is willing to stretch the meaning of subsystem. This leads us to the definition of a *partial* subsystem. In the context of classical CG it is hardly worth the effort but the goal here is to prepare the ground for quantum CG. The raw notion of CG does not land naturally in quantum theory, but it easily sneaks in as marginalization of a partial subsystem.

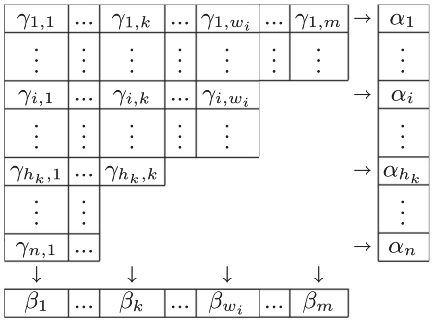
Consider the state space of a composite system AB that is the Cartesian product $\mathsf{C} := \mathsf{A} \times \mathsf{B}$, where $\mathsf{A} := \{\alpha_i\}_{i=1}^{|\mathsf{A}|}$ and $\mathsf{B} := \{\beta_k\}_{k=1}^{|\mathsf{B}|}$ are the state spaces of individual subsystems (now both α_i and β_k refer to microstates). Probabilistic states p_{C} live in the vector space $\mathbb{R}^{\mathsf{C}}$, and marginalization of subsystem A is given by the map $\mathcal{M} : \mathbb{R}^{\mathsf{A}\times\mathsf{B}} \longrightarrow \mathbb{R}^{\mathsf{B}}$ which accounts for our ignorance of system A. The map $\mathcal{M}$ is defined by the relation

$$p_{\mathsf{B}}(\beta) = \sum_{\alpha \in \mathsf{A}} p_{\mathsf{C}}(\alpha \times \beta).$$

The resemblance between this equation and Eq. (1) is obvious. If we partition C into blocks $\{\alpha \times \beta\}_{\alpha \in A}$ for each $\beta \in \mathsf{B}$, and slightly abuse the notation by also referring to each block with β, then CG as defined by Eq. (1) marginalizes A, and the action of CG matrix M is identical to that of map $\mathcal{M}$.

Marginalization is a special case of CG where all blocks are of the same size. In general this is not the case, but if we happen to partition a system (not necessarily composite) into blocks of equal size, we can think about it as a composite

TABLE I. Bipartition table. Arrows point toward the associated states of partial subsystems.



system of two *virtual* subsystems. Consider the state space $\mathsf{C} := \{\gamma_{ik}\}$ where the indices $i = 1 \ldots n$ and $k = 1 \ldots m$ define a partition of C into m blocks of n elements each. We then can imagine systems $\mathsf{A} := \{\alpha_i\}_{i=1}^{n}$ and $\mathsf{B} := \{\beta_k\}_{k=1}^{m}$ and identify the states $\gamma_{ik} \equiv \alpha_i \times \beta_k$ so $\mathsf{C} \cong \mathsf{A} \times \mathsf{B}$. Such subsystems are commonly known as *virtual subsystems*. Coarse graining with respect to this partition is effectively a marginalization of the virtual subsystem A.

In general we can specify any partition of $\mathsf{C} := \{\gamma_{ik}\}$ by assignment of indices i,k, where k refers to the block and i to the relative position of elements inside the block. It is convenient to order the blocks by descending block size and arrange the elements $\{\gamma_{ik}\}$ into what we call a *bipartition table* (Table I). The columns of this table correspond to CG blocks. If all blocks are of the same size, then the table is rectangular and the set of columns (rows) is associated with states of the virtual subsystems B (A), as indicated by the arrows. When the blocks are not all of the same size, the ranges of indices i,k are not independent from each other. If $k = 1 \ldots m$ for a fixed m, then $i = 1 \ldots h_k$ where h_k is the size of block k (height of column k). We can always invert the dependence so if $i = 1 \ldots n$, then $k = 1 \ldots w_i$ (width of row i). Even when the table is not rectangular, we can still associate the columns (rows) with states of fictitious system B (A), and identify $\gamma_{ik} \equiv \alpha_i \times \beta_k$ as composite states. We call such fictitious subsystems *partial subsystems.* What sets them apart from virtual subsystems is the fact that certain combinations of states are not allowed. The injective map $V : \mathsf{C} \longrightarrow \mathsf{A} \times \mathsf{B}$, which assigns elements of C into the bipartition table, will be called a *partial bipartition map* (the bipartition is not partial if V is bijective).

Marginalization of a partial subsystem is essentially the same procedure as marginalization of the nonpartial subsystem. We sum the probabilities over the rows or the columns of the bipartition table and assign them to reduced states. The fact that some combinations of composite states are not allowed simply means that they contribute nothing to the sums. To make this more rigorous, consider the partial bipartition map $V : \mathsf{C} \longrightarrow \mathsf{A} \times \mathsf{B}$. By applying V on the corresponding basis of $\mathbb{R}^{\mathsf{C}}$ we get the isomorphic embedding $\mathcal{V} : \mathbb{R}^{\mathsf{C}} \longrightarrow \mathbb{R}^{\mathsf{A}\times\mathsf{B}}$. The map $\mathcal{V}$ embeds probabilistic states of C into a subspace of probabilistic states of AB, spanned by the allowed combinations of states. Marginalizing with $\mathcal{M} : \mathbb{R}^{\mathsf{A}\times\mathsf{B}} \longrightarrow \mathbb{R}^{\mathsf{B}}$ after embedding with $\mathcal{V}$ defines the marginalization of the partial subsystem A:

$$\mathcal{M}\mathcal{V} : \mathbb{R}^{\mathsf{C}} \longrightarrow \mathbb{R}^{\mathsf{B}}.$$

Intuitively, the map $\mathcal{V}$ completes the missing blocks of the bipartition table to make it rectangular and assigns zero probability to the missing states. Then $\mathcal{M}$ sums the probabilities over the columns and assigns them to the associated states of B. Thus, $\mathcal{M}\mathcal{V}$ sums the probabilities over the columns of the bipartition table which means that $\mathcal{M}\mathcal{V}$ implements a CG of C according to the blocks defined by the columns of the table.

To recap, every system admits a partial bipartition into partial subsystems. Partial bipartition is defined by the shape of the bipartition table and the assignment of elements into it. Columns (rows) of the bipartition table are associated with states of partial subsystem B (A). We saw that marginalization of a partial subsystem is equivalent to CG over the columns. The fact that every CG is a marginalization of a partial subsystem is easy to see: just arrange the CG blocks into columns of a bipartition table with arbitrary ordering inside the blocks. Thus, CG can be equivalently defined as marginalization of a partial subsystem. This definition has a bit of extra structure that is not strictly necessary for classical CG. The extra structure is in the bipartition table which assigns order to elements inside the blocks (columns) and it is irrelevant if we simply sum over them.

It turns out that in the quantum version of marginalization—the partial trace—this ordering makes a difference. This also explains why we could not directly export CG into quantum theory from the basic definitions of Sec. II A. While partition into blocks provides enough structure to specify a CG for the classical state space, we need the extra structure of the bipartition table to specify a CG for the quantum state space.

III. QUANTUM COARSE GRAINING

The fundamental feature of quantum systems that sets them apart from their classical analogs is the superposition principle [17]. Therefore, for a notion of coarse graining to be truly "quantum," we must embrace the superposition principle and allow the possibility of reducing superpositions of microstates into superpositions of macrostates. Section III A is dedicated to the formal definition of such notion.

Although the definition of quantum CG (QCG) is quite simple, the interpretation requires some effort. We will show that just like in the classical case, QCG is a manifestation of restricted access to observables. The main technical result behind it is the definition of *bipartition operators*. In Sec. III B we will demonstrate this formalism in some special cases.

Section III C addresses the question of reducibility of dynamics. The problem is formulated in terms of a compatibility condition between a QCG scheme and a generator of dynamics. We will see that the general condition for compatibility can be derived and presented in exactly the same form as in the classical case. This result is then specialized to unitary quantum dynamics by Theorem 3.

In Sec. III D we focus on symmetries and the associated QCGs. Symmetry considerations have been fundamental in the development of many important ideas in physics: from Emmy Noether's seminal work [18] relating conserved quantities to the symmetries of dynamics, to the modern applications in

subjects ranging from crystallography [19] to error avoidance strategies in quantum computers [20]. Many of the applications of symmetries, including Noether's theorem, are concerned with their implications for dynamical processes. Therefore, the analysis of reducibility of dynamics would not be complete without introducing symmetry considerations. The main result that we derive in that regard is Theorem 4, where we specialize the compatibility condition to QCGs by symmetrization. This compatibility condition turns out to be a relaxed version of symmetry of dynamics, where the commutator $[U(g), H]$ may not vanish, but it has to belong to the operator algebra spanned by the group.

We end this section with an example of continuous-time quantum walk on a tree. It shows that symmetries can be used to reduce the dynamics even when they do not commute with the Hamiltonian.

A. Formal definitions

The difficulty with direct adoption of the classical notion of CG, in the quantum setting, arises because the classical notion is ignorant of the possibility of superpositions between the states. Consider a finite-dimensional Hilbert space as a quantized version of the classical state space, where microstates α_i were promoted to orthonormal basis $|\alpha_i\rangle$. If we partition the microstates into blocks $\{|\alpha_i\rangle\}_{i\in b}$, it may still make sense to say that all states $|\psi_b\rangle$ that belong to the span of block b are indistinguishable and should be reduced as $|\psi_b\rangle \longmapsto |b\rangle$. However, if we look at superpositions such as $|\psi\rangle = |\psi_b\rangle + |\psi_{b'}\rangle$, this CG reduction is not consistently defined. If we naively suggest that $|\psi\rangle \longmapsto |b\rangle + |b'\rangle$, then we can always write the same state differently, $|\psi\rangle = e^{i\varphi}|\tilde{\psi}_b\rangle + |\psi_{b'}\rangle$ where $|\tilde{\psi}_b\rangle := e^{-i\varphi}|\psi_b\rangle$, and get a different reduced state $|\psi\rangle \longmapsto e^{i\varphi}|b\rangle + |b'\rangle$.

Reduction of coherence terms between the blocks is simply undefined by the classical CG procedure. If we insist on using the classical notion as it is, the only sensible approach is to discard the coherence terms altogether. That is, the reduction of $|\psi\rangle = |\psi_b\rangle + |\psi_{b'}\rangle$ should be $|\psi\rangle \longmapsto |b\rangle\langle b| + |b'\rangle\langle b'|$. Such CG of quantum states is consistently defined, but it is not truly quantum.

For the truly quantum notion of CG we have to consistently account for coherence terms between the CG blocks. In order to do that, we will adopt a different perspective. Recall that classical CG was eventually understood as marginalization of a (partial) subsystem. This observation is key, because it shifts the focus from blocks and states to subsystems. Thus, quantum coarse graining can be introduced as quantum marginalization of a partial subsystem. Since the notion of quantum marginalization—the partial trace map—already exists, all we have left is to identify partial subsystems in the quantum setting.

It should be noted that mathematically equivalent definitions of the QCG map have been presented in Refs. [9] and [7]. Our definition is different in that it is derived by a direct analogy with the classical case. Furthermore, we will expand on the formal structure of QCG by identifying *bipartition operators* as key mathematical objects and *bipartition tables* as their graphical representation. We will also provide QCG with operational meaning.

1. Partial subsystems and bipartitions

Consider a finite-dimensional physical Hilbert space $\mathcal{H}$. The choice of orthonormal basis $\{|\gamma_{ik}\rangle\}$ and their arrangement into a bipartition table (Table I) constitutes a partial bipartition of $\mathcal{H}$. The auxiliary Hilbert space $\mathcal{H}^A$ ($\mathcal{H}^B$) of the partial subsystem A (B) is formally defined as the span of row kets $\{|\alpha_i\rangle\}_{i=1}^n$ (column kets $\{|\beta_k\rangle\}_{k=1}^m$) as illustrated in Table I. The physical Hilbert space $\mathcal{H}$ can now be isometrically embedded into the subspace of $\mathcal{H}^{AB} := \mathcal{H}^A \otimes \mathcal{H}^B$ with the map $V : |\gamma_{i,k}\rangle \longmapsto |\alpha_i\rangle|\beta_k\rangle$. For every $|\gamma_{i,k}\rangle \in \mathcal{H}$ there is a matching pair $|\alpha_i\rangle|\beta_k\rangle \in \mathcal{H}^{AB}$, but not vice versa. The extra pairs in $\mathcal{H}^{AB}$ that do not have a match in $\mathcal{H}$ correspond to the missing elements of the bipartition table that would complete it to a rectangular form. The case where the chosen bipartition table of $\mathcal{H}$ is rectangular, so $\mathcal{H} \cong \mathcal{H}^{AB}$, is the case where $\mathcal{H}^A$ and $\mathcal{H}^B$ were identified by [10] as *virtual* subsystems. The construction here is more general; therefore we refer to such subsystems as *partial* subsystems.

In the following it will be useful to express the isometry V in two complementary forms

$$V = \sum_{k=1}^{m} V_k^A \otimes |\beta_k\rangle = \sum_{i=1}^{n} |\alpha_i\rangle \otimes V_i^B. \tag{10}$$

The partial isometries

$$V_k^A := \sum_{i=1}^{h_k} |\alpha_i\rangle\langle\gamma_{i,k}|, \quad V_i^B := \sum_{k=1}^{w_i} |\beta_k\rangle\langle\gamma_{i,k}| \tag{11}$$

map the individual columns (rows) of the bipartition table into $\mathcal{H}^A$ ($\mathcal{H}^B$).

2. Quantum coarse graining map

Once the partial subsystem A is identified, QCG is defined as the map that traces out A. Since the partial trace map tr_A acts on operators, we have to elevate the action of the isometry V to operators as well, thus defining $\mathcal{V}(\cdot) := V(\cdot)V^\dagger$. Then, the composition

$$\mathrm{tr}_{(A)} := \mathrm{tr}_A \circ \mathcal{V}$$

defines the QCG map $\mathrm{tr}_{(A)}$. Since both components of this composition are completely positive trace preserving (CPTP) maps, QCG map $\mathrm{tr}_{(A)}$ reduces proper quantum states to proper quantum states [21]. Operator sum representation of $\mathrm{tr}_{(A)}$ can be obtained by expressing V in the second form of Eq. (10) and applying tr_A:

$$\mathrm{tr}_{(A)}(\rho) = \mathrm{tr}_A(V\rho V^\dagger) = \sum_{i=1}^{n} V_i^B \rho\, V_i^{B\dagger}.$$

Reduction with $\mathrm{tr}_{(A)}$ maps the density matrices between the operator spaces as

$$\mathrm{tr}_{(A)} : \mathcal{B}(\mathcal{H}) \longrightarrow \mathcal{B}(\mathcal{H}^A \otimes \mathcal{H}^B) \longrightarrow \mathcal{B}(\mathcal{H}^B),$$

so the partial subsystem B embodies the reduced, coarse-grained state space.

The choice of notation $\mathrm{tr}_{(A)}$ for the QCG map is justified by its action on the matrix elements in the bipartition basis $|\gamma_{i,k}\rangle$

$$\mathrm{tr}_{(A)} : |\gamma_{i,k}\rangle\langle\gamma_{j,l}| \longmapsto \delta_{ij}|\beta_k\rangle\langle\beta_l|. \tag{12}$$

So it traces over the indices i, j as if they label basis elements of a proper subsystem (the bracketed subscript $_{(A)}$, as opposed to the unbracketed one $_A$, refers to the fact that it traces over a *partial* subsystem).

As an illustration, consider the 6-dimensional Hilbert space $\mathcal{H}$ spanned by the orthonormal basis $\{|s\rangle\}$ for $s = 1, \ldots, 6$. A partial bipartition of $\mathcal{H}$ is chosen such that in the basis $\{|s\rangle\}$ it is specified by the bipartition table

1	2	3
4	5	
6		

We will now use the notation $|\gamma_{i,k}\rangle$ to refer to the same elements $|s\rangle$ by their row and column indices, for example $|4\rangle \equiv |\gamma_{2,1}\rangle$.

An arbitrary pure state can then be written as $|\psi\rangle = |\psi_1\rangle + |\psi_2\rangle + |\psi_3\rangle$, where each unnormalized state $|\psi_i\rangle$ is the support of $|\psi\rangle$ on the row i:

$$
\begin{aligned}
|\psi_1\rangle &:= c_{11}|\gamma_{1,1}\rangle + c_{12}|\gamma_{1,2}\rangle + c_{13}|\gamma_{1,3}\rangle,\\
|\psi_2\rangle &:= c_{21}|\gamma_{2,1}\rangle + c_{22}|\gamma_{2,2}\rangle,\\
|\psi_3\rangle &:= c_{33}|\gamma_{3,1}\rangle.
\end{aligned}
$$

Applying Eq. (12) on the element $|\psi_i\rangle\langle\psi_j|$ we get

$$
\mathrm{tr}_{(A)}(|\psi_i\rangle\langle\psi_j|) = \delta_{ij}\sum_{k,l} c_{ik}\overline{c_{il}}|\beta_k\rangle\langle\beta_l|.
$$

Then if we present the density matrix $\rho := |\psi\rangle\langle\psi|$ in the bipartition basis ordered by their appearance in the bipartition table (read from left to right and top to bottom), the action of $\mathrm{tr}_{(A)}$ is

$$
\begin{pmatrix}
\rho_{11} & \rho_{12} & \rho_{13} & \rho_{14} & \rho_{15} & \rho_{16}\\
\rho_{21} & \rho_{22} & \rho_{23} & \rho_{24} & \rho_{25} & \rho_{26}\\
\rho_{31} & \rho_{32} & \rho_{33} & \rho_{34} & \rho_{35} & \rho_{36}\\
\rho_{41} & \rho_{42} & \rho_{43} & \rho_{44} & \rho_{45} & \rho_{46}\\
\rho_{51} & \rho_{52} & \rho_{53} & \rho_{54} & \rho_{55} & \rho_{56}\\
\rho_{61} & \rho_{62} & \rho_{63} & \rho_{64} & \rho_{65} & \rho_{66}
\end{pmatrix}
$$

$$
\downarrow \mathrm{tr}_{(A)}
$$

$$
\begin{pmatrix}
\rho_{11}+\rho_{44}+\rho_{66} & \rho_{12}+\rho_{45} & \rho_{13}\\
\rho_{21}+\rho_{54} & \rho_{22}+\rho_{55} & \rho_{23}\\
\rho_{31} & \rho_{32} & \rho_{33}
\end{pmatrix}
$$

The colored blocks (color online) of the top matrix correspond to the elements $|\psi_i\rangle\langle\psi_i|$. From this we learn how to "read" the action of QCG from the bipartition table:

(1) Coherences between basis elements $|\gamma_{i,k}\rangle\langle\gamma_{j,l}|$ in different rows ($i \neq j$) of the bipartition table are discarded.

(2) For each pair of columns k,l (including $k = l$), the sum of coherences between $|\gamma_{i,k}\rangle\langle\gamma_{i,l}|$ over all rows i is the new coherence term for the reduced element $|\beta_k\rangle\langle\beta_l|$.

The original Hilbert space can then be decomposed to sectors

$$
\mathcal{H} = \bigoplus_{k=1}^{m} \mathcal{H}_k, \tag{13}
$$

where $\mathcal{H}_k$ is the span of elements in column k of the bipartition table. This decomposition is analogous to the partition of the classical state space to blocks. The rule 2 above suggests that a state supported on a single column $\mathcal{H}_k$ collapses into a macrostate $|\beta_k\rangle$, as in the classical case. Similarly, all statistical mixtures of states supported on different columns collapse into statistical mixtures of the corresponding macrostates. The quantum-classical similarities end when we consider superpositions between the blocks. QCG attempts to reduce the coherence terms between the blocks into a single coherence term between the corresponding macrostates, but it cannot do so perfectly. The result is potentially diminished coherence between the macrostates of the reduced state.

Although the visual representation of QCG in terms of columns and rows of the bipartition table is appealing, its operational meaning is not clear. In the following we will identify a set of operators that capture the structure of the bipartition table and use them to gain insight about QCG's operational meaning.

3. Bipartition operators

Similarly to how we obtained the operator sum representation of $\mathrm{tr}_{(A)}$, we can obtain another representation by using the first form of V in Eq. (10):

$$
\begin{aligned}
\mathrm{tr}_{(A)}(\rho) &= \mathrm{tr}_A(V\rho V^\dagger)\\
&= \mathrm{tr}_A\left[\left(\sum_{l=1}^{m} V_l^A \otimes |\beta_l\rangle\right)\rho\left(\sum_{k=1}^{m} V_k^{A\dagger} \otimes \langle\beta_k|\right)\right]\\
&= \sum_{k,l=1}^{m} \mathrm{tr}\left[V_k^{A\dagger} V_l^A \rho\right]|\beta_l\rangle\langle\beta_k|.
\end{aligned}
$$

This brings us to the definition of the bipartition operators

$$
S_{kl} := V_k^{A\dagger} V_l^A = \sum_{i=1}^{\min(h_k,h_l)} |\gamma_{i,k}\rangle\langle\gamma_{i,l}| \tag{14}
$$

that map between columns of the bipartition table by preserving the row index i of each element (the element is eliminated if the row is not present in the destination column).

As a result, we obtain a different representation of the QCG map (in Ref. [22] such representation of quantum channels is described as input-output, or tomographic representation):

$$
\mathrm{tr}_{(A)}(\rho) = \sum_{k,l} \mathrm{tr}(S_{kl}\rho)|\beta_l\rangle\langle\beta_k|. \tag{15}
$$

Since the bipartition operators can be read directly from the bipartition table, from now on we will use the right-hand side of Eqs. (14) and (15) as the defining constructs of QCG and leave the isometry V behind (the bipartition table is of course still the underlying structure from which all of these constructs are derived).

In order to obtain the operational meaning of QCG, consider what observable information is preserved in the reduced state. Formally, the information in the reduced state $\rho_B := \mathrm{tr}_{(A)}(\rho)$ predicts, according to Born's rule, the expectation values $\mathrm{tr}(O_B\rho_B)$ for all observables O_B in $\mathcal{O}(\mathcal{H}^B)$ (the set of observables on B). Since Born's rule is identical to the Hilbert-Schmidt (HS) inner product $\langle O_B, \rho_B\rangle_{HS} := \mathrm{tr}(O_B^\dagger\rho_B)$, we can lift the QCG map from states and apply it to

observables,

$$\mathrm{tr}(O_B\rho_B) = \langle O_B, \mathrm{tr}_{(A)}(\rho)\rangle_{HS} = \langle \mathrm{tr}^\dagger_{(A)}(O_B), \rho\rangle_{HS},$$

where $\mathrm{tr}^\dagger_{(A)}$ is the Hermitian adjoint of $\mathrm{tr}_{(A)}$ with respect to the HS inner product (the same symbol † for Hermitian adjoint will be used for both operators and superoperators). The following set of observables on the original (unreduced) system,

$$\mathcal{O}^B(\mathcal{H}) := \{\mathrm{tr}^\dagger_{(A)}(O_B) \,|\, O_B \in \mathcal{O}(\mathcal{H}^B)\} \subset \mathcal{O}(\mathcal{H}), \tag{16}$$

consists of all the observables whose expectation values are preserved by QCG.

The explicit form of $\mathrm{tr}^\dagger_{(A)}$ can be derived by rearranging the traces and sums in

$$\begin{aligned}\langle O_B, \mathrm{tr}_{(A)}(O)\rangle_{HS} &= \mathrm{tr}\left(O_B^\dagger \sum_{k,l} \mathrm{tr}(S_{kl}O)|\beta_l\rangle\langle\beta_k|\right)\\ &= \mathrm{tr}\left(\sum_{k,l} S_{kl}\mathrm{tr}(O_B^\dagger|\beta_l\rangle\langle\beta_k|)O\right)\\ &= \left\langle\left(\sum_{k,l} S_{kl}\langle\beta_k|O_B^\dagger|\beta_l\rangle\right)^\dagger, O\right\rangle_{HS}.\end{aligned}$$

Then, using $S_{kl} = S^\dagger_{lk}$ and rearranging the indices, we get

$$\mathrm{tr}^\dagger_{(A)}(O_B) = \sum_{k,l} S_{kl}\langle\beta_k|O_B|\beta_l\rangle. \tag{17}$$

It is now clear that $\mathcal{O}^B(\mathcal{H}) \subset \mathsf{span}\{S_{kl}\}$. Conversely, for every observable $O \in \mathsf{span}\{S_{kl}\}$ we can find an $O_B \in \mathcal{O}(\mathcal{H}^B)$ such that $O = \mathrm{tr}^\dagger_{(A)}(O_B)$. Therefore, bipartition operators S_{kl} span the operator subspace containing all and only the observables preserved by QCG. Then we can interpret the coarse-grained state ρ_B as the state that contains all and only the information that is accessible to observer restricted to $\mathsf{span}\{S_{kl}\}$. The QCG map can then be understood as a change-of-observer transformation.

In the familiar case of tensor product bipartition $\mathcal{H} = \mathcal{H}^A \otimes \mathcal{H}^B$, bipartition operators take the form

$$S_{kl} := I_A \otimes |\beta_k\rangle\langle\beta_l|.$$

The restricted set of observables $\mathsf{span}\{S_{kl}\} = I_A \otimes \mathcal{B}(\mathcal{H}^B)$ implies that the observer can only measure system B. The QCG map (15) specializes to the usual tr_A and the reduced states $\mathrm{tr}_A(\rho)$ represent what the restricted observer can actually "see." In Sec. III B we will see other familiar state transformations that can be understood as special cases of QCG.

This closes the circle with the classical picture of CG from which we started. Classical CG was introduced as the manifestation observer's inability to distinguish some states, which is in fact a restriction of observational power. Now we see that both classical and quantum notions admit the same operational interpretation: CG is the result of restricted observational ability.

4. Generalization: Quantum-classical hybrid

With bipartition operators it is easy to extend the quantum notion of CG to include the original classical one. Intermediate notions, which combine both classical and quantum features, are quick to follow (we will keep referring to them as QCG). This generalization will allow us to associate QCG with symmetries in Sec. III D.

The purely classical notion of CG can be imported into quantum state space by simply disregarding the coherence terms. Using the set $\{\Pi_k\}$ of projections on sectors $\mathcal{H} = \bigoplus_{k=1}^m \mathcal{H}_k$ that specify the classical blocks, the classical CG map is defined as

$$\rho \longmapsto \sum_k \mathrm{tr}(\Pi_k\rho)|\beta_k\rangle\langle\beta_k|. \tag{18}$$

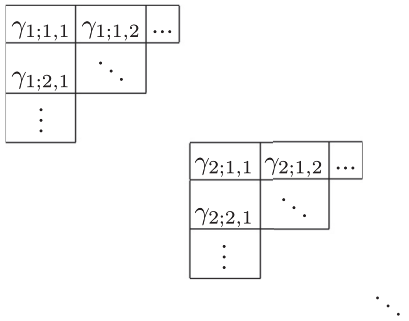
One can always represent probability vectors as diagonal density matrices and use this map to implement classical CG as defined by Eq. (1). Comparing Eq. (18) to the quantum version (15) suggests that the set of projections $\{\Pi_k\}$ is the classical equivalent of the bipartition operators. In fact, note that by definition (14), bipartition operators of the form S_{kk} are projections on sectors. If we think of bipartition operators as k,l elements of some matrix, then S_{kk} are the diagonal elements. Classical CG can then be thought of as a restriction of some QCG specified by $\{S_{kl}\}$ to the diagonal elements $\{S_{kk}\}$.

This perspective leaves room for intermediate cases that arise from restriction of the complete set $\{S_{kl}\}$ to block diagonal elements. It is convenient to introduce the index q to refer to the blocks of bipartition operators, such that $\{S_{q,kl}\}_{kl}$ is a block diagonal set with k,l running over the elements of block q. The hybrid CG map is then specified by the set $\{S_{q,kl}\}$ and it acts similarly to (15),

$$\rho \longmapsto \sum_{q,k,l} \mathrm{tr}(S_{q,kl}\rho)|\beta_{q,l}\rangle\langle\beta_{q,k}|, \tag{19}$$

with the addition of index q. The purely quantum case is when q specifies a single block, making the index q unnecessary. The purely classical case is when each block q has only one bipartition operator: the projection Π_q. The truly hybrid case selects the supersectors $\mathcal{H} = \bigoplus_q \mathcal{H}_q$ of the Hilbert space where each subset $\{S_{q,kl}\}_{kl}$ of bipartition operators is supported. The map (19) reduces each supersector $\mathcal{H}_q$ into a distinct sector in the reduced state space while discarding all coherence terms between the different $\mathcal{H}_q$.

We can also generalize the visual representation of QCG with bipartition tables by allowing block diagonal arrangements of cells. For each subset of operators $\{S_{q,kl}\}_{kl}$ we have a block of cells in the bipartition table, and the different blocks live on the diagonal of the full table:



This arrangement results in the block diagonal set $\{S_{q,kl}\}$ if we use the original construction (14) of bipartition operators with such tables.

B. Special cases of the coarse-graining map

The general QCG map (19) captures a lot of common state manipulations—which are not usually thought of as CG—as its special cases. Since the QCG map is completely specified by the set of bipartition operators it is possible to capture the key structure associated with such manipulations in the neat visual form of the bipartition table. In the following we point out a few of such state manipulations.

For concreteness we will consider the system of two or more spin-$\frac{1}{2}$ particles:

$$\mathcal{H} := \left(\mathcal{H}^{(\frac{1}{2})}\right)^{\otimes N}, \quad \mathcal{H}^{(\frac{1}{2})} = \mathsf{span}\{|\uparrow\rangle,|\downarrow\rangle\}.$$

Change of basis. The trivial QCG that does not actually loose any information may still change the basis in which the density matrix is presented. The change of basis map, disguised as QCG, is specified by arranging the new basis elements into a single row of the bipartition table. For 2 spins, changing to the total spin basis $|j,m\rangle$ is given by the table

$1,1$	$1,0$	$1,-1$	$0,0$

which specifies the bipartition operators

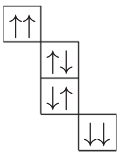
$$S_{j,m;j',m'} := |j,m\rangle\langle j',m'|,$$

where j,m are used to refer to the columns of the table. The QCG map then simply changes the basis

$$\begin{aligned}\rho &\longmapsto \sum_{j,m;j',m'} \mathrm{tr}(S_{j,m;j',m'}\rho)|j',m'\rangle\langle j,m| \\ &= \sum_{j,m;j',m'} \langle j',m'|\rho|j,m\rangle|j',m'\rangle\langle j,m|.\end{aligned}$$

This should make clear the fact that the result of any QCG, even the trivial one, depends on the choice of basis that go into the bipartition table.

Projective measurement. Projective measurements, up to the readout of the outcome, can be thought of as purely classical CGs. Here the bipartition table has a column-diagonal form and the columns are specified by the projections on the outcomes. For 2 spins, the QCG resulting from measurement of the total spin z component (without reading the outcome) is specified by the table



There are only 3 bipartition operators defined by this table: the projections

$$\begin{aligned}S_{1,1} &= |\uparrow\uparrow\rangle\langle\uparrow\uparrow|, \\ S_{0,0} &= |\uparrow\downarrow\rangle\langle\uparrow\downarrow| + |\downarrow\uparrow\rangle\langle\downarrow\uparrow|, \\ S_{-1,-1} &= |\downarrow\downarrow\rangle\langle\downarrow\downarrow|,\end{aligned}$$

where $j_z = 1,0,-1$ are used to label the columns. The associated QCG map

$$\rho \longmapsto \sum_{j_z=-1,0,1} \mathrm{tr}\big(S_{j_z,j_z}\rho\big)|j_z\rangle\langle j_z|$$

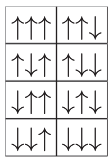
results in a diagonal matrix containing the probability distribution over the three outcomes.

Tensor product structures and (virtual) subsystems. Illustrating bipartite tensor product structures is where the bipartition table really simplifies the picture. The natural tensor product structure of the Hilbert space of 2 spins A and B is captured by the bipartition table

It is arranged such that the degrees of freedom of spin A are constant inside the rows and the degrees of freedom of spin B are constant inside the columns. This table defines the bipartition operators $S_{kl} := I \otimes |k\rangle\langle l|$ for $k,l = \uparrow,\downarrow$ and the associated QCG map is just the partial trace over A (rotate the table by 90° to get the partial trace over B):

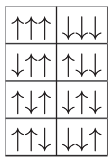
$$\begin{aligned}\rho &\longmapsto \sum_{k,l=\uparrow,\downarrow} \mathrm{tr}(I \otimes |k\rangle\langle l|\rho)|l\rangle\langle k| \\ &= \sum_{k,l=\uparrow,\downarrow} \mathrm{tr}(|k\rangle\langle l|\mathrm{tr}_A(\rho))|l\rangle\langle k| = \mathrm{tr}_A(\rho).\end{aligned}$$

For 3 spins we can consider the first 2 spins as subsystem A and the third spin as subsystem B. Arranging the bipartition table where B's degrees of freedom are constant inside the columns and A's inside the rows results in



which specifies a QCG map that traces out the first 2 spins. By rearranging this table we can specify different (possibly virtual) bipartite tensor product structures.

For example



specifies the natural tensor product structure of the repetition code. The virtual subsystem associated with the columns now encodes the logical qubit, while the virtual subsystem associated with the rows encodes the syndrome. The 4 bipartition operators consist of 2 projections S_{00}, S_{11} on the columns (0, 1 label the two columns), and 2 isometries S_{01}, S_{10} between the columns that exchange elements inside the rows [recall Eq. (14) for explicit definition]. A single spin flip error X_i acts on the top row—the code space—by translating it to the $i+1$ row, so

$$\begin{aligned}S_{kl}X_i|\uparrow\uparrow\uparrow\rangle &= X_i S_{kl}|\uparrow\uparrow\uparrow\rangle, \\ S_{kl}X_i|\downarrow\downarrow\downarrow\rangle &= X_i S_{kl}|\downarrow\downarrow\downarrow\rangle.\end{aligned}$$

Therefore, for any encoding $|\psi\rangle = \alpha|\uparrow\uparrow\uparrow\rangle + \beta|\downarrow\downarrow\downarrow\rangle$ we can have a single spin flip error that will not affect the

coarse-grained state:

$$\begin{aligned} X_i|\psi\rangle\langle\psi|X_i \longmapsto & \sum_{k,l=0,1} \mathrm{tr}(S_{kl}X_i|\psi\rangle\langle\psi|X_i)|l\rangle\langle k| \\ = & \sum_{k,l=0,1} \mathrm{tr}(S_{kl}|\psi\rangle\langle\psi|)|l\rangle\langle k| \\ = & \ (\alpha|0\rangle+\beta|1\rangle)(\overline{\alpha}\langle 0|+\overline{\beta}\langle 1|). \end{aligned}$$

In this context we think of the QCG map as a decoding procedure that traces out the syndrome degrees of freedom and produces the encoded qubit.

Reference frames and noiseless subsystems. For errors that arbitrarily change the reference frame (RF) there are *noiseless subsystems* where information can be encoded in RF-independent degrees of freedom [20]. Such degrees of freedom can be associated with the reduced state that is seen by an observer that does not have access to the RF in which the state was prepared [23]. This reduction of state can also be considered as QCG.

Since RFs are completely specified by a group of transformations that change them, the relevant structure of QCG is selected by the irreducible representations of the group (we will elaborate on this in Sec. III D). Considering a system of three spins and a RF of direction associated with global rotations, we get the bipartition table

$\frac{3}{2},+\frac{3}{2}$		
$\vdots$		
$\frac{3}{2},-\frac{3}{2}$		
	$\frac{1}{2},+\frac{1}{2},0$	$\frac{1}{2},+\frac{1}{2},1$
	$\frac{1}{2},-\frac{1}{2},0$	$\frac{1}{2},-\frac{1}{2},1$

There are two blocks in this table corresponding to the irreducible representations of total spin $\frac{3}{2}$ and $\frac{1}{2}$. The block of total spin $\frac{1}{2}$ specifies the virtual tensor product $|\frac{1}{2},\pm\frac{1}{2}\rangle\otimes|k\rangle$ where $k=0,1$ labels the two copies of this representation. The 5 bipartition operators specified by this table are

$$S_{\frac{3}{2}} := \sum_{j_z=-\frac{3}{2},\ldots,\frac{3}{2}} \left|\frac{3}{2},j_z\right\rangle\!\left\langle\frac{3}{2},j_z\right| = I^{(\frac{3}{2})},$$

$$S_{\frac{1}{2},kl} := \sum_{j_z=-\frac{1}{2},\frac{1}{2}} \left|\frac{1}{2},j_z,k\right\rangle\!\left\langle\frac{1}{2},j_z,l\right| = I^{(\frac{1}{2})}\otimes|k\rangle\langle l|,$$

and, according to Schur's lemmas [19], they span the space of all operators that commute with all global rotations that act on $(\mathcal{H}^{(\frac{1}{2})})^{\otimes 3}$. Therefore, according to the operational interpretation of QCG, the reduced state retains only the information accessible with rotationally invariant measurements. Such restriction of measurements is what defines the observer that has no access to the RF of direction [23] so this QCG produces the effective state that such observer can see.

In the context of noiseless subsystems we can say that such QCG "traces out" rotationally noninvariant degrees of freedom and produces the qubit encoded in the rotationally invariant degrees of freedom.

C. Compatibility with dynamics

As was discussed in the classical case, the coarse-grained state may fail to follow a well-defined dynamical rule. The dynamics in the coarse-grained state space may be such that it is impossible to tell, from the initial conditions alone, where the system will go. The situation is essentially the same as the one we see in open quantum systems (see [13] or [11] for a comprehensive review). In fact it was recently shown [7] that under dimension-reducing maps, such as our QCG map, the reduced dynamics can be described in the same way we describe the dynamics of open quantum systems. This conclusion should also be evident from the approach to QCG we have developed here: if QCG is a marginalization of a (partial) subsystem then the remaining subsystem should evolve as an open quantum system. This means that in general the evolution may not be universal, so the dynamical map that governs the evolution is different for different initial conditions and may not be completely positive [11]. Even when the dynamics are universal we may still lose the semigroup structure which allows us to characterize the dynamics with generators.

How to deal with these difficulties in the context of open quantum systems is an area of active research [24] and we will not attempt to address it here. Our situation is different in that we have the freedom to choose the bipartition that may be compatible with the given dynamics. Instead of asking how a fixed subsystem evolves, we ask how to choose a (partial) subsystem so it evolves in a nice way. This question will be now addressed in the form of compatibility condition between QCGs and dynamics.

The way the compatibility condition was derived in the classical case (Sec. II B) is sufficiently general to be reproduced in the quantum setting. The classical condition $PQ=PQP$ of Theorem 1 has two components: the generator of dynamics Q and the CG projection P. Since the QCG map $\mathrm{tr}_{(A)}$ is a superoperator that acts on density matrices, the quantum analogs of Q and P must also be superoperators. The analog of Q is the Lindblad superoperator $\mathcal{L}$ [11,13], which generates time evolutions of the density matrix ρ as the solutions of

$$\frac{d}{dt}\rho = \mathcal{L}(\rho). \tag{20}$$

This equation is the quantum analog of Eq. (5).

The QCG projection can be defined identically to its classical analog $P=M^+M$ as

$$\mathcal{P} := \mathrm{tr}^+_{(A)}\circ\mathrm{tr}_{(A)}, \tag{21}$$

where $\mathrm{tr}^+_{(A)}$ is the Moore-Penrose pseudoinverse of the QCG map $\mathrm{tr}_{(A)}$. The explicit form of this pseudoinverse is not necessary for our purposes and we will only use its defining properties and the fact that it exists (all finite-dimensional linear operators—including $\mathrm{tr}_{(A)}$—have one). For the sake of completeness we will present the explicit forms of $\mathrm{tr}^+_{(A)}$ and $\mathcal{P}$ after proving Lemma 1 bellow.

With these definitions Theorem 1 can be reproduced in the quantum setting by replacing P with $\mathcal{P}$, Q with $\mathcal{L}$, M (M^+) with $\mathrm{tr}_{(A)}$ ($\mathrm{tr}^+_{(A)}$), probability vectors with density matrices, and Eq. (5) with Eq. (20). The proof is the same because it relies on the linear algebraic properties of the operators (which in

both cases are assumed to be finite-dimensional matrices) and nothing more. The result is that

$$\mathcal{P}\mathcal{L} = \mathcal{P}\mathcal{L}\mathcal{P} \tag{22}$$

is the quantum compatibility condition in the general form. When this condition holds, and only then, the reduced state $\rho_B := \mathrm{tr}_{(A)}(\rho)$ evolves according to

$$\frac{d}{dt}\rho_B = \tilde{\mathcal{L}}(\rho_B),$$

where $\tilde{\mathcal{L}} = \mathrm{tr}_{(A)} \circ \mathcal{L} \circ \mathrm{tr}^{+}_{(A)}$.

The compatibility condition in its general form (22) is quite opaque. In the classical case it was Corollary 1 that provided some insight into how to find compatible CG by looking at transition rates. Extracting similar insight for quantum dynamics is not as easy. We will not address this general case here but we will specialize the generator $\mathcal{L}$ to unitary dynamics (given by a Hamiltonian) and reformulate the condition (22) in a more transparent way. In the next subsection we will specialize this condition further by focusing on QCGs given by a group representation.

The first step in clarifying the condition (22) is finding out the operator subspace on which $\mathcal{P}$ projects.

Lemma 1. Let $\{S_{kl}\}$ be a set of bipartition operators, and let $\mathcal{P}$ be the associated coarse-graining projection as defined by Eq. (21). Then $\mathcal{P}$ is an orthogonal projection on the operator subspace $\mathsf{span}\{S_{kl}\}$.

Proof. The defining properties of the Moore-Penrose pseudoinverse [12] imply that the map $\mathcal{P}$ is an orthogonal projection on the subspace orthogonal to the kernel of $\mathrm{tr}_{(A)}$, that is, $\mathsf{im}(\mathcal{P}) = \mathsf{ker}(\mathrm{tr}_{(A)})^{\perp}$. Next, to see that $\mathsf{ker}(\mathrm{tr}_{(A)})^{\perp} = \mathsf{span}\{S_{kl}\}$, we will apply $\mathrm{tr}_{(A)}$ on S_{kl}. Using the action (12) on the definition (14) we get

$$\mathrm{tr}_{(A)}(S_{kl}) = \mathsf{min}(h_k, h_l)|\beta_k\rangle\langle\beta_l|. \tag{23}$$

From this we see that the image of $\mathsf{span}\{S_{kl}\}$ under $\mathrm{tr}_{(A)}$ is the whole $\mathsf{im}(\mathrm{tr}_{(A)})$. The minimal subspace with such property is $\mathsf{ker}(\mathrm{tr}_{(A)})^{\perp}$; therefore $\mathsf{ker}(\mathrm{tr}_{(A)})^{\perp} \subseteq \mathsf{span}\{S_{kl}\}$. On the other hand, every nonzero operator in $\mathsf{span}\{S_{kl}\}$ does not vanish under $\mathrm{tr}_{(A)}$; therefore $\mathsf{span}\{S_{kl}\} \subseteq \mathsf{ker}(\mathrm{tr}_{(A)})^{\perp}$. The two mutual inclusions then imply

$$\mathsf{span}\{S_{kl}\} = \mathsf{ker}(\mathrm{tr}_{(A)})^{\perp} = \mathsf{im}(\mathcal{P}).$$

■

Now we note that the pseudoinverse $\mathrm{tr}^{+}_{(A)}$ is a map from $\mathsf{im}(\mathrm{tr}_{(A)})$ to $\mathsf{ker}(\mathrm{tr}_{(A)})^{\perp}$, that is,

$$\mathrm{tr}^{+}_{(A)} : \mathsf{span}\{|\beta_k\rangle\langle\beta_l|\} \to \mathsf{span}\{S_{kl}\}.$$

Equation (23) suggests that for the inverse property $\mathrm{tr}_{(A)} \circ \mathrm{tr}^{+}_{(A)} = \mathcal{I}$ to hold we must have $\mathrm{tr}^{+}_{(A)}(|\beta_k\rangle\langle\beta_l|) = \mathsf{min}(h_k, h_l)^{-1} S_{kl}$ which defines the pseudoinverse

$$\mathrm{tr}^{+}_{(A)}(O_B) = \sum_{kl} \frac{\langle\beta_k|O_B|\beta_l\rangle}{\mathsf{min}(h_k, h_l)} S_{kl}.$$

This map can be seen as a composition of $\mathrm{tr}^{\dagger}_{(A)}$ [see Eq. (17)] with rescaling by $\mathsf{min}(h_k, h_l)$.

The explicit form of $\mathcal{P} = \mathrm{tr}^{+}_{(A)} \circ \mathrm{tr}_{(A)}$ is then given by acting with $\mathrm{tr}^{+}_{(A)}$ on Eq. (15):

$$\begin{aligned}\mathcal{P}(O) &= \sum_{k,l} \mathrm{tr}(S_{kl} O)\mathrm{tr}^{+}_{(A)}(|\beta_l\rangle\langle\beta_k|) \\ &= \sum_{k,l} \frac{\mathrm{tr}(S_{kl} O)}{\mathsf{min}(h_k, h_l)} S_{lk}.\end{aligned}$$

It should be noted that even though the QCG $\mathrm{tr}_{(A)}$ maps states to states (is CPTP), we cannot claim that $\mathrm{tr}^{+}_{(A)}$ and $\mathcal{P}$ have this property in general. Nonetheless, the QCG projection $\mathcal{P}$ is a useful formal construct that captures the compatibility condition (22) and its properties will be used in the proof of Theorem 3.

In the following we will use the fact that $\mathcal{P}$ is an *orthogonal* projection, as stated by Lemma 1, meaning that not only $\mathcal{P}^2 = \mathcal{P}$ but also $\mathcal{P}^{\dagger} = \mathcal{P}$ [the Hermitian adjoint is defined with respect to the HS inner product $\langle \mathcal{P}(A), B\rangle_{HS} = \langle A, \mathcal{P}^{\dagger}(B)\rangle_{HS}$].

Now we will assume unitary dynamics. This means that the generator $\mathcal{L}$ is of the form $-i[H, \cdot]$, where H is the Hamiltonian. The following theorem expresses the compatibility condition (22) in terms of H and $\{S_{kl}\}$.

Theorem 3. Let $\mathcal{L}(\cdot) := -i[H, \cdot]$ be a generator of dynamics with Hamiltonian H, and let $\{S_{kl}\}$ be bipartition operators that specify a coarse graining. Then, the compatibility condition (22) is equivalent to

$$[H, S] \in \mathsf{span}\{S_{kl}\}, \quad \forall S \in \mathsf{span}\{S_{kl}\}.$$

Proof. First we note that $\mathcal{L}$ is an anti-Hermitian superoperator: $\mathcal{L}^{\dagger} = -\mathcal{L}$. This can be shown explicitly:

$$\begin{aligned}\langle A, \mathcal{L}(B)\rangle_{HS} &= \mathrm{tr}(A^{\dagger}(-i[H, B])) \\ &= \mathrm{tr}(-i A^{\dagger} H B) + \mathrm{tr}(i A^{\dagger} B H) \\ &= \mathrm{tr}(-i A^{\dagger} H B) + \mathrm{tr}(i H A^{\dagger} B) \\ &= \mathrm{tr}(-\mathcal{L}(A)^{\dagger} B) = \langle -\mathcal{L}(A), B\rangle_{HS}.\end{aligned}$$

By taking the Hermitian adjoint on both sides of (22), and using the fact that $\mathcal{P}^{\dagger} = \mathcal{P}$, we get

$$-\mathcal{L}\mathcal{P} = -\mathcal{P}\mathcal{L}\mathcal{P} = -\mathcal{P}\mathcal{L}.$$

The compatibility condition is then equivalent to

$$\mathcal{L}\mathcal{P} = \mathcal{P}\mathcal{L}.$$

Lemma 1 implies that for any $S \in \mathsf{span}\{S_{kl}\}$ we have $\mathcal{P}(S) = S$ and $\mathcal{P}(O) \in \mathsf{span}\{S_{kl}\}$ for any O. Therefore,

$$[H, S] = i\mathcal{L}(S) = i\mathcal{L}\mathcal{P}(S) = i\mathcal{P}\mathcal{L}(S) \in \mathsf{span}\{S_{kl}\}.$$

For the opposite direction we assume that $i\mathcal{L}(S) = [H, S] \in \mathsf{span}\{S_{kl}\}$ for any $S \in \mathsf{span}\{S_{kl}\}$. Since $\mathcal{P}$ is an orthogonal projection on $\mathsf{span}\{S_{kl}\}$, for any O we have $\mathcal{L}\mathcal{P}(O) \in \mathsf{span}\{S_{kl}\}$, which implies $\mathcal{L}\mathcal{P} = \mathcal{P}\mathcal{L}\mathcal{P}$. ■

D. Coarse graining and symmetries

As was discussed in the classical case, symmetrizing the states can also be considered as CG. We will now reproduce this argument for the quantum case and utilize it to address the question of reducibility of dynamics.

Our construction relies on structures selected by irreducible representations (irreps) of the group and the associated operator algebras. Developments in fault-tolerant quantum computation [25–27], the study of quantum reference frames and the emergence of superselection rules [23,28], and more recently quantification of the notion of asymmetry [29,30] have all contributed to the establishment of the algebraic framework that we will use here.

We begin by recalling Hilbert space decompositions induced by representations of groups [19]. Given a finite or a compact Lie group G, with the unitary representation $U(G)$ on the Hilbert space $\mathcal{H}$, there is a decomposition

$$\mathcal{H} = \bigoplus_{q,n} \mathcal{M}_{q,n} \cong \bigoplus_{q} \mathcal{M}_q \otimes \mathcal{N}_q. \tag{24}$$

The sectors $\mathcal{M}_{q,n}$ carry irreps of the group, the index q runs over the inequivalent irreps, and n labels the different occurrences of the same irrep. The isomorphism on the right follows by "collecting" all the equivalent irreps into a tensor product of the virtual subsystems $\mathcal{M}_q$ (the irrep space) and $\mathcal{N}_q$ (the multiplicity space). Then, the group action can be expressed in the form

$$U(g) = \bigoplus_{q} U_{\mathcal{M}_q}(g) \otimes I_{\mathcal{N}_q}, \tag{25}$$

where $U_{\mathcal{M}_q}(g)$ are irreducible unitary representations of the group action. This explicitly shows that the group acts by transforming all $\mathcal{M}_q$ independently according to the irrep q, while leaving all $\mathcal{N}_q$ unaffected.

The structure (24) selected by the group (from here on, by "group" we refer to the group of unitary operators acting on the Hilbert space, not the abstract representationless group) can now be used to implement a QCG. For an isolated sector q, tracing over the virtual subsystem $\mathcal{M}_q$ can be seen as a QCG given by the bipartition operators

$$S_{q,kl} := I_{\mathcal{M}_q} \otimes |q,k\rangle\langle q,l|, \tag{26}$$

where $|q,k\rangle$ are some arbitrary orthonormal basis of $\mathcal{N}_q$. The combined set (for all q) of bipartition operators $\{S_{q,kl}\}$ specifies a hybrid notion of QCG as defined by Eq. (19).

Such QCG will be called *coarse graining by symmetrization* because it eliminates all information in the asymmetric degrees of freedom. In order to see that explicitly, consider the commutant algebra of the group, defined by

$$U(G)' := \{B \in \mathcal{B}(\mathcal{H}) \,|\, [B, U(g)] = 0,\ \forall g \in G\}.$$

It is an immediate consequence of Schur's lemmas, and the group action (25), that $U(G)'$ consists of all operators of the form

$$B = \bigoplus_{q} I_{\mathcal{M}_q} \otimes B_{\mathcal{N}_q}. \tag{27}$$

Compare it to Eq. (26), from which follows $U(G)' = \mathsf{span}\{S_{q,kl}\}$. Since the loss of information under QCG is captured by orthogonal projection on $\mathsf{span}\{S_{q,kl}\}$, it then follows that the information that is eliminated in this case resides in the degrees of freedom that are not invariant under the action of the group.

So far we have established that unitary representations of groups can be used to specify a QCG scheme. The question remaining is which groups are useful for the reduction of dynamics. Historically, the groups that are considered in the study of dynamical processes are the ones that commute with the dynamics. In the case of unitary time evolutions, these are the groups that commute with the Hamiltonian $[U(g), H] = 0$. In this case $H \in U(G)'$ so it can be expressed in the form (27)

$$H = \bigoplus_{q} I_{\mathcal{M}_q} \otimes H_{\mathcal{N}_q}. \tag{28}$$

Dynamics generated by such Hamiltonians keep the irrep spaces $\mathcal{M}_q$ stationary, while evolving the multiplicity spaces $\mathcal{N}_q$ independently in each sector. Therefore, the degrees of freedom associated with the irrep spaces $\mathcal{M}_q$ can be safely ignored when considering time evolutions. From this we conclude that QCG by symmetrization with the symmetry group of the Hamiltonian is compatible with dynamics. [This can be shown rigorously by invoking the compatibility condition of Theorem 3 and using the fact that $H \in U(G)' = \mathsf{span}\{S_{q,kl}\}$.]

This however, does not mean that symmetries of the Hamiltonian are the only groups that are useful for the reduction of dynamics. The appropriate generalization of symmetries of the Hamiltonian, capturing all groups that can be used to reduce the dynamics, is given in the following theorem.

Theorem 4. Let G be a finite or a compact Lie group with unitary representation $U(G)$ on $\mathcal{H}$. Then, coarse graining by symmetrization with $U(G)$ is compatible with dynamics generated by the Hamiltonian H if and only if

$$[U(g), H] \in U(G)'', \quad \forall g \in G, \tag{29}$$

where $U(G)''$ is the commutant of $U(G)'$.

Proof. Using the fact that the bipartition operators $\{S_{q,kl}\}$ of QCG by symmetrization span $U(G)'$, we can express the compatibility condition of Theorem 3 as

$$[H, B] \in U(G)', \quad \forall B \in U(G)'.$$

By definition of $U(G)'$, this is equivalent to

$$[U(g), [H, B]] = 0, \quad \forall B \in U(G)', \forall g \in G.$$

Since $[U(g), B] = 0$, we can rearrange the Lie bracket

$$[[U(g), H], B] = 0, \quad \forall B \in U(G)', \forall g \in G.$$

But this means that for all g, $[U(g), H]$ must be in the commutant of $U(G)'$, so

$$[U(g), H] \in U(G)'', \quad \forall g \in G.$$

Since it is equivalent to the condition of Theorem 3, which is necessary and sufficient, it is also necessary and sufficient. ■

The commutant $U(G)''$ of the algebra $U(G)'$ consists of all operators of the form [25]

$$A = \bigoplus_{q} A_{\mathcal{M}_q} \otimes I_{\mathcal{N}_q}.$$

Since all $U(g)$ are of this form, that is $U(g) \in U(G)''$, condition (29) implies that groups such that $H \in U(G)''$ are compatible. Symmetries of the Hamiltonian, for which $H \in U(G)'$, trivially comply with the condition (29) because $0 \in U(G)''$. In general, the compatibility condition (29) implies a very specific form for the Hamiltonian.

Proposition 2. Any operator H that complies with the condition (29) is of the form

$$H = A + B = \bigoplus_q \left(A_{\mathcal{M}_q} \otimes I_{\mathcal{N}_q} + I_{\mathcal{M}_q} \otimes B_{\mathcal{N}_q}\right), \qquad (30)$$

where $A \in U(G)''$ and $B \in U(G)'$.

Proof. Condition (29) implies that for every $g \in G$ there is an $A_g \in U(G)''$ such that

$$U(g)HU(g)^\dagger - H = A_g.$$

Rearranging the terms and integrating over G (summing for finite groups) with an invariant measure $d\mu(g)$ we get

$$H = \underbrace{-\int_G d\mu(g) A_g}_{A} + \underbrace{\int_G d\mu(g) U(g) H U(g)^\dagger}_{B}.$$

We have $A \in U(G)''$ by definition of A_g, and $B \in U(G)'$ because of the invariance of the measure $d\mu(g) = d\mu(g')$ (or rearrangement theorem for finite groups). ■

It is now easy to see why groups that comply with condition (29) lead to compatible QCG by symmetrization. The form (30) implies that the subsystems $\mathcal{M}_q$ and $\mathcal{N}_q$ do not interact with each other. The explicit form of the time evolution operator is

$$U_H(t) = e^{-itH} = \bigoplus_q e^{-itA_{\mathcal{M}_q}} \otimes e^{-itB_{\mathcal{N}_q}},$$

so each part of the virtual composite system $\mathcal{M}_q \otimes \mathcal{N}_q$ evolves independently from the other. Therefore, we can generate time evolutions in $\mathcal{N}_q$ without having to know the state of $\mathcal{M}_q$ (and vise versa), and that is the defining property needed for the reduction of dynamics.

Symmetries of the Hamiltonian ($[U(g), H] = 0$) are too restrictive for the purposes of reduction of dynamics. They require that, in addition to subsystem $\mathcal{N}_q$ evolving independently, subsystem $\mathcal{M}_q$ must be stationary, which is not necessary. Relaxing the condition to (29), and letting $\mathcal{M}_q$ evolve leads to a broader set of groups, beyond symmetries of the Hamiltonian. Thus, Theorem 4 provides us with more possibilities to confine the dynamical evolutions to smaller state spaces.

For practical applications it is beneficial to express the compatibility condition (29) in terms of the generators of the group. Assuming $\{L_\alpha\}$ are the generators of $U(G)$, and using the group action near the identity $U(\epsilon_\alpha) = I - \epsilon_\alpha i L_\alpha$ (for finite groups we can use the generators directly), the compatibility condition becomes

$$[L_\alpha, H] \in U(G)'', \quad \forall L_\alpha.$$

Furthermore, the operator algebra $\mathsf{Alg}\{L_\alpha\}$, of all polynomials in $\{L_\alpha\}$, is a subalgebra of $U(G)''$ [by definition of $U(G)'$, every L_α must commute with everything in $U(G)'$]. Thus, replacing $U(G)''$ with $\mathsf{Alg}\{L_\alpha\}$ results in the sufficient condition

$$[L_\alpha, H] \in \mathsf{Alg}\{L_\beta\}, \quad \forall L_\alpha.$$

E. Example: Continuous-time quantum walk on a binary tree

Continuous-time quantum walk (CTQW) is a generic model of quantum dynamics that admits visually intuitive demonstration of QCG by symmetrization. More specifically, we will focus on CTQW on binary trees introduced by [31] and demonstrated to evolve in a reduced state space in Ref. [32].

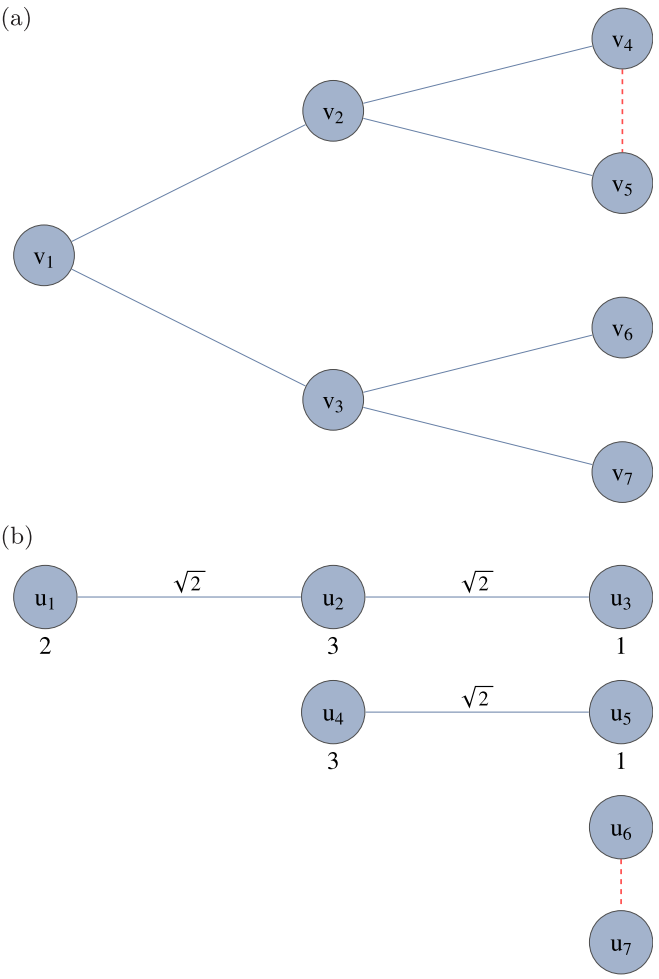


FIG. 5. Quantum walk on a tree (a) is reduced to parallel quantum walks over the columns of the tree (b). Labels on the edges indicate transition rates and labels under the vertices indicate local potentials (the default value is 1 for both). Addition of the red dashed edge in (a) results in the addition of identical edge in (b). Even though the red edge breaks the symmetry of the tree it does not affect the reduced dynamics between the columns (see main text).

The CTQW model is specified by a simple undirected graph $\mathcal{G}$ with vertices V and edges E. The Hilbert space is defined as $\mathcal{H} := \mathsf{span}\{|v_i\rangle\}_{v_i \in V}$, and the Hamiltonian is constructed in the same way as the stochastic transition rates matrix (in this case all rates are normalized to 1):

$$H := -\sum_{(v_i, v_j) \in E} (|v_i\rangle\langle v_j| + |v_j\rangle\langle v_i|) + \sum_{v_i \in V} d_i |v_i\rangle\langle v_i|. \qquad (31)$$

The degree d_i of a vertex v_i is the total number of vertices connected to it.

The concrete example we will analyze is shown in Fig. 5(a), where we ignore the red dashed line for now and focus on the tree spanned by the solid edges. If this was a classical random walk, then CG by partition of vertices to the 3 columns would be compatible with dynamics. In the quantum case,

however, partition to sectors is not enough to specify a CG, and there is not much else to guide us in the appropriate choice of compatible bipartition other than symmetries.

Symmetries of CTQWs arise from the automorphisms of the underlying graph [33]. Graph automorphisms form a group $\mathsf{Aut}_{\mathcal{G}} := \{\varphi\}$ that consists of permutations of vertices that leave the set of edges unchanged

$$(v_i, v_j) \in E \Leftrightarrow (v_{\varphi(i)}, v_{\varphi(j)}) \in E.$$

Using the cycle notation for permutations, our graph automorphisms are generated by $a = (45)$ and $b = (23)(47)(56)$; it is also instructive to point out the group element $c = bab = (67)$. Permutation b can be thought of as a flip of the whole tree around the horizontal axes through the root, while permutations a and c are flips of the subtrees around horizontal axes through their own roots.

In order to streamline the calculations, it is convenient to express the Hamiltonian as a sum of permutations. Permutations are naturally represented by orthogonal (unitary) operators

$$\Pi_\varphi := \sum_i |v_{\varphi(i)}\rangle\langle v_i|.$$

The Hamiltonian (31) can now be written as a sum of 2-cycle permutations (ij) (note that $\Pi_{(ij)}$ acts as the identity on vertices that are not v_i or v_j):

$$H = -\sum_{(v_i,v_j)\in E} \Pi_{(ij)} + |E|I.$$

Since $|E|I$ only adds a total phase to the evolutions we can safely drop it. In our concrete case the Hamiltonian is

$$H = -\Pi_{(12)} - \Pi_{(13)} - \Pi_{(24)} - \Pi_{(25)} - \Pi_{(36)} - \Pi_{(37)}. \quad (32)$$

Note that the adjoint action of any permutation φ on a 2-cycle results in another 2-cycle:

$$\Pi_\varphi \Pi_{(ij)} \Pi_\varphi^T = \Pi_{(\varphi(i)\varphi(j))}.$$

It is now easy to check that the group generated by $a = (45)$ and $b = (23)(47)(56)$ commutes with the Hamiltonian, because the adjoint action of Π_a or Π_b permutes the 2-cycles in Eq. (32), but leaves the whole sum unchanged:

$$\Pi_a H \Pi_a^T = \Pi_b H \Pi_b^T = H.$$

Therefore, the finite group $\mathsf{Aut}_{\mathcal{G}}$ represented by the unitary operators $\{\Pi_a, \Pi_b\}$ is a symmetry of the Hamiltonian.

Using the shorthand notation

$$|+_{ijk\ldots}\rangle = \frac{|v_i\rangle + |v_j\rangle + |v_k\rangle + \cdots}{\text{normalization}},$$
$$|\pm_{ijk\ldots}\rangle = \frac{|v_i\rangle - |v_j\rangle + |v_k\rangle - \cdots}{\text{normalization}},$$

we first identify the 3 trivial irreps of $\mathsf{Aut}_{\mathcal{G}}$ as the subspaces

$$\mathcal{M}_{1,1} := \mathsf{span}\{|+_1\rangle\},$$
$$\mathcal{M}_{1,2} := \mathsf{span}\{|+_{23}\rangle\},$$
$$\mathcal{M}_{1,3} := \mathsf{span}\{|+_{4567}\rangle\}.$$

There are also 2 nontrivial but equivalent irreps, where Π_a acts by 1 and Π_b acts by -1:

$$\mathcal{M}_{2,1} := \mathsf{span}\{|\pm_{23}\rangle\},$$
$$\mathcal{M}_{2,2} := \mathsf{span}\{|\pm_{4657}\rangle\}.$$

The last irrep is single and 2-dimensional:

$$\mathcal{M}_3 := \mathsf{span}\{|\pm_{4567}\rangle, |\pm_{5467}\rangle\}.$$

Accounting for multiplicities, the Hilbert space decomposes to

$$\mathcal{H} = (\mathcal{M}_1 \otimes \mathcal{N}_1) \oplus (\mathcal{M}_2 \otimes \mathcal{N}_2) \oplus \mathcal{M}_3,$$

where $\mathcal{N}_1$ and $\mathcal{N}_2$ are 3 and 2 dimensional multiplicity spaces. Now we can change to the new bases $|u_i\rangle$ that are native to these irreps:

$$|u_1\rangle := |+_1\rangle, \quad |u_4\rangle := |\pm_{23}\rangle, \quad |u_6\rangle := |\pm_{4567}\rangle,$$
$$|u_2\rangle := |+_{23}\rangle, \quad |u_5\rangle := |\pm_{4657}\rangle, \quad |u_7\rangle := |\pm_{5467}\rangle,$$
$$|u_3\rangle := |+_{4567}\rangle.$$

In the new bases the Hamiltonian is block diagonal $H = H_1 \oplus H_2 \oplus H_3$, where

$$H_1 = \begin{pmatrix} 2 & -\sqrt{2} & 0 \\ -\sqrt{2} & 3 & -\sqrt{2} \\ 0 & -\sqrt{2} & 1 \end{pmatrix},$$
$$H_2 = \begin{pmatrix} 3 & -\sqrt{2} \\ -\sqrt{2} & 1 \end{pmatrix}, \quad (33)$$
$$H_3 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

(We added back the global term $|E|I$ to present the more conventional diagonal elements.) This is the explicit form (28) of H that acts nontrivially on multiplicity spaces only. The terms H_1, H_2 act on multiplicity spaces of 1-dimensional irreps, and the term H_3 acts trivially because $\mathcal{M}_3$ is multiplicity free. Therefore, the dynamics can be isolated as quantum walks on disconnected components associated with the irreps; see Fig. 5(b). One complication that arises, caused by boundaries of the finite graph, is the nonconstant potential on the vertices, as seen on the diagonal of the Hamiltonian.

Quantum walk in the multiplicity space of the trivial irrep [top row in Fig. 5(b)] was first shown in Ref. [32] to be the reduced 1D walk over the "column states" ($|u_1\rangle$, $|u_2\rangle$, $|u_3\rangle$ in our notation). Boundary effects, causing a potential "bump," were numerically shown to be not significant in the larger trees. More importantly, it was understood that the reduced quantum walk on the 1D chain of "column states" is responsible for the exponential speedup in propagation time from the leafs to the root, compared to the classical walk. Note however that the full speedup occurs only from the initial state $|u_3\rangle$. If the initial state is also supported on $|u_5\rangle$ then the speedup will only carry it to the second column, and if it had support on $|u_6\rangle$ or $|u_7\rangle$ then those parts are stuck in the initial column.

The insight is that the reduced dynamics of quantum walks on trees persist even if the symmetry of the tree is broken in a manner that is described by Eq. (29). Adding the red dashed edge to the tree in Fig. 5(a) breaks the original automorphism symmetry since $(v_4, v_5) \in E$ but $(v_{b(4)}, v_{b(5)}) = (v_7, v_6) \notin E$. The new Hamiltonian H', when expressed as a sum of 2-cycles, receives an additional term $H' = H - \Pi_{(45)}$, which breaks the

symmetry under the action of b:

$$\Pi_b H' \Pi_b^T = H - \Pi_{(76)} \neq H'.$$

The action of $a = (45)$, however, still commutes with H'. The commutator of H' with Π_b can be expressed as

$$[\Pi_b, H'] = [\Pi_b, H] - [\Pi_b, \Pi_a] = [\Pi_a, \Pi_b],$$

so it belongs to the operator algebra spanned by the generators $\{\Pi_a, \Pi_b\}$. Theorem 4 then implies that QCG by such symmetrization is still compatible with dynamics. The only difference is that in addition to acting on the multiplicity spaces, the Hamiltonian may act independently on the irreps. In this case, only $\mathcal{M}_3$ can be affected (dynamics in 1-dimensional irreps are absorbed into the multiplicity spaces). Even though $|u_i\rangle$ are now native to irreps of a group that is not a symmetry of the Hamiltonian, we can still use them to block-diagonalize the Hamiltonian. The new decomposition is $H' = H_1 \oplus H_2 \oplus H_3'$ where H_1, H_2 are the same as before (33), and

$$H_3' = \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}.$$

H_3' generates nontrivial evolutions in $\mathcal{M}_3$ which can be seen graphically as addition of the red dashed edge in Fig. 5(b). It generates evolutions vertically, in a stationary subspace of the right column, but it does not interfere with dynamics across the columns.

This example demonstrates the fact that strict symmetries of the Hamiltonian are not necessary for the effective reduction of dynamics. That being said, it is not easy to see *a priori* which groups are compatible. This would not work, for example, if we broke the symmetry with $\Pi_{(56)}$ instead of $\Pi_{(45)}$, since $[\Pi_{(56)}, \Pi_a]$ is not an element in the operator algebra spanned by $\{\Pi_a, \Pi_b\}$. Just because $\Pi_{(56)}$ generates dynamics within the column does not mean that it cannot interfere with the dynamics across the columns. In our case, the choice of $\Pi_{(45)}$ to break the symmetry works, because it is the element a of the symmetry group of the Hamiltonian. Since $\mathsf{Aut}_{\mathcal{G}}$ is not Abelian, the modified Hamiltonian was no longer commuting with it, but because the symmetry-breaking element came from the group, the commutant was guaranteed to be in the operator algebra spanned by the group.

IV. SUMMARY AND OUTLOOK

We have established the common notion of coarse graining in both classical and quantum settings and provided it with operational meaning. By introducing bipartition tables we were able to capture the key structure of a coarse-graining scheme in a concise, visual form. Our main focus—the reduction of dynamics by coarse-graining the state space—led to the formulation of compatibility conditions between a coarse-graining scheme and dynamics. Such compatibility conditions were shown to be necessary and sufficient for the existence of a reduced generator of dynamics that governs time evolutions in the coarse-grained state space. Considering symmetrizations of states with a group representation as a special case of coarse graining, and specializing the compatibility condition to this case, we showed how group representations can be used to reduce the dynamics. This result turned out to be closely related to Noether's theorem that uses symmetries of dynamics to identify the static degrees of freedom, i.e., constants of motion. We generalized this perspective with less restricted group representations to identify dynamically independent degrees of freedom. Such degrees of freedom are not necessarily constants of motion and the group representations are not necessarily symmetries of dynamics.

The task of reducing dynamics that was studied here demands an exact reproduction of dynamical evolutions in the reduced state space. The only way to satisfy such demand is to single out the degrees of freedom that evolve independently from the rest. As we pointed out, finding group representations that satisfy the commutation relation (29) is one possible approach to the problem of exact reduction. This formulation, however, might be too strict for some practical application and an approximate reduction may be in order. The compatibility conditions for the exact reduction can then be taken as a starting point for the development of approximations when the conditions are not exactly satisfied.

Aside from the reduction of dynamics, the notion of coarse graining raises some interesting questions on its own. QCG was shown to be the map that accounts for some ignorance of the observer. Specifically, it accounts for the restriction to measurements that belong to the span of bipartition operators that define the QCG scheme. Such restricted observers arise naturally in physical situations characterized by inability to measure external environment, or inaccessibility of a particular reference frame in which the system is prepared. The QCG formalism allows us to account for all these and more general restrictions, but the physical situations that lead to the more general cases are not so clear. In particular, we can now account for restrictions to observables that do not form an algebra: the general span of bipartition operators is an *operator system.* Then the question is, what physical situations lead to the restriction to observables that form an operator system, but not an algebra?

Regardless of physical interpretations, QCG is a powerful analytical concept that offers flexible ways to "select" quantum information encoded in the physical state. Within the framework of QCG we can capture information selected by group representations, virtual subsystems, and restricted observables under the same umbrella concept. We believe that this generic nature makes QCG a fundamental concept of quantum information with potential applications in quantum error correction, tomography, and quantum thermodynamics.

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