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Spectrum for some quantum Markov semigroups describing N-particle systems evolving under a binary collision mechanism

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Abstract. We compute the spectrum for a class of quantum Markov semigroups describing systems of N particle interacting through a binary collision mechanism. These quantum Markov semigroups are associated to a novel kind of quantum random walk on a graph, with the graph structure arising naturally in the quantization of the classical Kac model, and we show that the spectrum of the generator of the quantum Markov semigroup is closely related to the spectrum of the Laplacian on the corresponding graph. For the direct analog of the original classical Kac model, we determine the exact spectral gap for the quantum generator. We also give a new and simple method for studying the spectrum of certain graph Laplacians.

1. Introduction

We study the rate of approach to equilibrium in a quantum version of the classical Kac model that was developed in [9]. The original Kac model [20, 21] concerns a dilute gas of N molecules interacting through pair-wise collision that conserve the energy, and in this model, the collision mechanism gives rise to a jump process on a continuous state space, the "energy sphere" of the N particles, and the Kolmogorov forward equation for this jump process is known as the *Kac Master Equation*.

Interactions between molecules are properly described by quantum mechanics, and the model introduced in [9] is a natural adaptation of Kac's classical model to the quantum setting, in which the Kac Master Equation becomes an equation of Lindblad type, the *Quantum Kac Master Equation* (QKME). The assumptions on the collision mechanism in [9] were rather general, and the paper concentrated on general features such as classifying the equilibrium states, proving propagation of chaos (see [9]) and studying the resulting non-linear quantum Boltzmann equation. Little was said about

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the actual evolution and about the spectral properties of the generator of the quantum Markov semigroup, which is the subject of this paper.

In the present work, we consider a special collision rule that is described below and which is the direct analog of the one first considered by Kac. This specificity allows a much more detailed analysis. As we show, the quantization leads to a graph structure on an orthonormal basis of eigenstates of the N-particle energy operator. We will give a complete description of the spectrum of the QKME generator in terms of spectrum of the graph Laplacian on this graph. This yields a description of the quantum evolution in terms of the eigenvectors of these graph Laplacians.

One may view the QKME as a quantum Kolmogorov forward equation for a sort of quantum random walk on the graph associated to the collision mechanism. However, this sort of quantum random walk is different from the class of random walks on graphs introduced by Aharonov, Ambainis, Kempe, and Vazirani [1]. In particular, the graph structure emerges naturally from the dynamics and is not present from the beginning. Of course, it is not surprising to see discrete mathematical structures emerging from quantization. Quantum Master Equations of the general type we investigate here do not only arise in quantum models of a gas of particles; they also arise in *random circuits* [17] and in the context of *measurement-only dynamics* [19].

In the model we focus on here, the graphs that arise turn out to be the closely connected with the *multislice* (see [16]), a natural generalization of the sliced Boolean cube. Recently proved ergodic properties of the random walk on slices of the multislice [15,16,24] then become relevant to QKME. However, the Kac model perspective sheds light on spectral analysis of Laplacians on graphs: we give a simple proof of the result of Caputo, Liggett, and Richthammer [5] that the spectral gap of the Laplacian on the multislice for N particles has the same value, namely, N, for all non-trivial connected components of the graph. This leads to an exact determination of the spectral gap for our quantum Kac model.

Section 2 gives an overview of classical and the quantum mechanical Kac model. In Section 3, the graph structure of the collision rules is explained, and here, we state our main result on the spectral gap of the QKME, giving an overview of the approach we will take. In Section 4, we work out the action of the QKME generator on a convenient orthonormal basis, which, while it does not consist of eigenvectors, leads to the identification of a family of invariant subspaces. The main result here is Theorem 4.1. Then, in Section 5, we apply Theorem 4.1 to reduce the spectral decomposition to the diagonalization of a graph Laplacian. In Section 6, the spectrum of the Laplacian on the collision graph is analyzed in detail, using methods adapted from our previous work in classical Kac Master Equations [6, 8, 9]. Finally, in Section 7, we briefly discuss some open problems concerning the use of relative entropy inequalities to control the rate of approach to equilibrium rather than spectral gaps.

2. Background on the quantum Kac model

2.1. The classical Kac model

The model investigated here is a quantum analog of a classical probabilistic model concerning a Markov jump process in a continuous state space. When the quantum analog is investigated, the "quantization" leads to interesting problems in discrete mathematics. To explain how these arise, we preface our investigation with a synopsis of the classical model.

The study of systems of colliding particles using master equations was initiated in 1956 by Mark Kac [20]. He invented a master equation describing a system of N particles in one dimension undergoing elastic pair collisions. The gas is spatially homogeneous which means that the state of the system is entirely described by the velocities of the N particles, given in $\vec{v} = (v_1, \ldots, v_N)$.

When a collision occurs, a random pair $1 \le m < n \le N$ is selected, and then, the velocities of particles m, n change from (v_m, v_n) to (v_m^*, v_n^*), where

$$v_m^* = v_m \cos\theta + v_n \sin\theta, \quad v_n^* = -v_m \sin\theta + v_n \cos\theta,$$

and all other velocities remain the same. The energy, $\frac{m}{2}\sum_{n=1}^{N} v_n^2$, is conserved by the collisions. Let $\mathcal{S}_{N,E}$ denote the sphere radius $\sqrt{E}$ in $\mathbb{R}^N$.

The "Kac walk" described below is a continuous time jump process in $\mathbb{R}^N$ with the jumps corresponding to collisions. Because of energy conservation, the collisions take points in $\mathcal{S}_{N,E}$ to points in $\mathcal{S}_{N,E}$, and hence, we may also consider it as a continuous time Markov jump process in $\mathcal{S}_{N,E}$, and if we seek ergodicity, we must restrict the process to an energy shell.

For $1 \le m, n \le N$, and $0 \le \theta < 2\pi$, define the map $R_{m,n}(\theta)$ on $\mathcal{S}_{N,E}$:

$$\big(R_{m,n}(\theta)\vec{v}\big)_k = \begin{cases} v_i \cos\theta + v_j \sin\theta, & k = i, \\ -v_i \sin\theta + v_j \cos\theta, & k = j, \\ v_k, & k \ne i, j. \end{cases} \tag{2.1}$$

In the original version of the Kac model, the angle θ is random with uniform distribution for simplicity. For $1 \le m < n \le N$, define an operator on continuous functions F on $\mathcal{S}_{N,E}$ by

$$\mathcal{Q}_{m,n} F(\vec{v}) = \frac{1}{2\pi}\int_0^{2\pi} F\big(R_{m,n}(\theta)\vec{v}\big)\mathrm{d}\theta. \tag{2.2}$$

The collision times arrive in a Poisson stream with mean waiting time $1/N$ which ensures that the mean waiting time for any particular particle to collide is of order one, uniformly in N. The evolution of the distribution of the particle velocities,

$F(v_1, \dots, v_N, t)$, is given by the Kac Master Equation (KME)

$$\partial_t F = \mathcal{L}_N F, \quad F(\cdot, 0) = F_0(\cdot),$$

where

$$\mathcal{L}_N F = N \binom{N}{2}^{-1} \sum_{m<n} (\mathcal{Q}_{m,n} - \mathbb{1}) F.$$

Moreover, it is easy to see that this walk is ergodic; i.e., the only equilibrium distribution is the uniform measure on $\mathcal{S}_{N,E}$, and that $\mathcal{L}_N$ is self-adjoint on $L^2(\mathcal{S}_{N,E})$, the Hilbert space of functions on $\mathcal{S}_{N,E}$ that are square integrable with respect to the uniform probability measure on $\mathcal{S}_{N,E}$.

It follows that if $F_0^{(N)}(v_1, \dots, v_N)$ is a probability density on $\mathcal{S}_{N,E}$, then

$$\lim_{t\to\infty} e^{t\mathcal{L}_N} F_0^{(N)} = 1, \tag{2.3}$$

the uniform probability density on $\mathcal{S}_{N,E}$. The rate at which this limit is approached is related to the rate of relaxation to equilibrium in a model Boltzmann equation, as Kac showed; see [9] for discussion. The rate of approach to equilibrium in (2.3) can be investigated by analyzing the spectral gap of the generator $\mathcal{L}_N$ (see [8]), as Kac originally proposed, or using entropy production inequalities (see [7, 25]). For the simple Kac model discussed here, the spectral gap is very well understood, though even in this case, there are still a number of open questions concerning entropy production.

2.2. The quantum Kac model

Here, we are concerned with a quantum analog of the classical Kac model described above. The state of a quantum system of N identical particles with finitely many degrees of freedom is given by a unit vector Ψ_N in the N-fold tensor product $\mathcal{H}_N := \otimes^N \mathcal{H}$ of a finite-dimensional Hilbert space $\mathcal{H}$, which is the state space for a single particle. Properly speaking, the state is actually the rank one projector onto the span of Ψ which is usually denoted by $|\Psi\rangle\langle\Psi|$. Such a state is called a *pure state*. More generally, the state may be described by an *ensemble* of pure states, that is, a convex combination

$$\varrho = \sum_{j=1}^{n} p_j |\Psi_j\rangle\langle\Psi_j|,$$

where each $p_j \geq 0$, and $\sum_{j=1}^n p_j = 1$ and each Ψ_j is a unit vector in $\mathcal{H}_N$. We do not assume that they are orthogonal, and there is no bound imposed on n. (One can even replace the sum by an integral.) The idea is that the actual state of the system is one of the pure states, but we do not know which one. We only know that it is Ψ_j with probability p_j. Evidently, the self-adjoint operator ϱ is positive semi-definite, and has

unit trace, that is, $\mathrm{Tr}[\rho] = 1$. Such operators are known as *density matrices*, and by the spectral theorem, every density matrix can be written in terms of an ensemble of pure states.

We now consider a random evolution of the quantum state ϱ corresponding to random binary collisions that conserve energy, as in the classical Kac model. The energy in the quantum setting is given by a self-adjoint operator known as the Hamiltonian. Suppose that the single particle Hamiltonian on $\mathcal{H}$ is given by a self-adjoint operator h. Define the N-particle Hamiltonian H_N on $\mathcal{H}_N$ as a sum of N terms

$$H_N = (h \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1}) + \cdots + (\mathbb{1} \otimes \cdots \otimes h \otimes \cdots \otimes \mathbb{1}) + \cdots + (\mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes h),$$

where $\mathbb{1}$ is the identity on $\mathcal{H}$, and where in the nth term, there is a single h which is in the nth position.

Now, we seek the quantum analog of the change in state corresponding to a single binary energy conserving collision such as $\vec{v} \mapsto R_{m,n}(\theta)\vec{v}$ with $R_{m,n}(\theta)$ given by (2.1). Suppose that, before the collision, the state of the system is given by a unit vector $\Psi \in \mathcal{H}_N$ such that $H_N \Psi_N = E \Psi_N$; that is, Ψ_N is an eigenstate of Hamiltonian with eigenvalue E. Physically, this means that Ψ is a state with a precisely defined energy E.

Though we are not keeping track of positions, one should imagine that, at some random time, particles m and n pass close to each other and interact. (This would be described by another part of the Hamiltonian, active only when two particles are sufficiently close.) After the collision, the new state has the form $U_{m,n}\Psi$, where $U_{m,n}$ is a unitary operator on $\mathcal{H}_N$ that could in principle be obtained by solving Schrödinger's equation for the full interacting Hamiltonian. The unitary $U_{m,n}$ will also depend on certain *collision parameters* corresponding to the relative positions of the particles during the collision, for example, whether it was merely a "grazing collision" or a "head on collision" or something in between. Position information is not encoded into Ψ, so these collision parameters will be external classical parameters. Hence, there will be a variety of possible unitaries $U_{m,n}(\sigma)$, σ belonging to some parameter space $\mathcal{C}$. Each $U(\sigma)$ is required to conserve the energy in the sense that $U_{m,n}(\sigma)H_N = H_N U_{m,n}(\sigma)$, which as usual we denote by writing

$$[U_{m,n}(\sigma), H_N] = 0.$$

Then, $U_{m,n}(\sigma)\Psi$ will be an eigenvector of H_N with eigenvalue E whenever Ψ is. We also require each $U_{m,n}$ to act non-trivially only on the mth and nth factors of $\mathcal{H}$ in $\mathcal{H}_N$.

To make this precise, first, consider the case $m = 1$ and $n = 2$. We begin with $N = 2$ and will then "lift" our constructions to the full N-particle model. Let $\mathcal{C}$ denote the group of unitaries on the 2 particle space $\mathcal{H}_2$ that commute with H_2. Throughout

the paper, we refer to $\mathcal{C}$ as the *collision group* of the model. Note that $\mathcal{C}$ is a compact Lie group. We regard the elements σ of $\mathcal{C}$ as representing all kinematically possible collisions of two particles. We now "lift" these collisions to the N-particle system. Define $U_{1,2}(\sigma)$ to be the unitary operator on $\mathcal{H}_N$ given by

$$U_{1,2}(\sigma)(\phi_1 \otimes \phi_2 \otimes \phi_3 \otimes \cdots \otimes \phi_N) = U(\sigma)(\phi_1 \otimes \phi_2) \otimes \phi_3 \otimes \cdots \otimes \phi_N,$$

where $U(\sigma)$ is the natural representation of $\sigma \in \mathcal{C}$ on $\mathcal{H}_2$. In the same way, for $1 \leq m < n \leq N$, we define $U_{m,n}$ so that it acts on the mth and nth factors of $\mathcal{H}$. The unitary $U_{m,n}$ describes the effects of a particular type of collision between particles m and n. Note that since $U(\sigma)$ commutes with H_2, $U_{m,n}(\sigma)$ commutes with H_N. The quantum analog of $\vec{v} \mapsto R_{m,n}(\theta)\vec{v}$ is then $\Psi \mapsto U_{m,n}(\sigma)\Psi$. Then, of course, $|\Psi\rangle\langle\Psi| \mapsto U_{m,n}(\sigma)|\Psi\rangle\langle\Psi|U^*_{m,n}(\sigma)$, or more generally,

$$\rho \mapsto U_{m,n}(\sigma)\rho U^*_{m,n}(\sigma).$$

To define the quantum analog of (2.2), we need to specify a probability law on the collision parameters σ. For some probability measure ν on $\mathcal{C}$, we define, for each $1 \leq m < n \leq N$, the operator $\mathcal{Q}_{m,n}$ on $\mathcal{B}(\mathcal{H}_N)$ by

$$\mathcal{Q}_{m,n}(X) = \int_{\mathcal{C}} U_{m,n}(\sigma) X U^*_{m,n}(\sigma) \mathrm{d}\nu(\sigma). \tag{2.4}$$

Throughout the paper, we refer to ν as the *collision law*, in the sense of a probability law, since it specifies the likelihood of the different possible collisions. The collision law may be supported on a measurable subset, in particular on a subgroup, of the collision group $\mathcal{C}$.

Equation (2.4) is the quantum analog of (2.2) except that of course ν needs to be specified. In the model actually investigated here, we take ν to be the normalized Haar measure on $\mathcal{C}$, which is the analog of the uniform measure on the planar rotation group that appears in (2.2). We can also consider other choices of ν, but they should have certain properties: we require that ν is invariant under the map $\sigma \mapsto \sigma^{-1}$ because this ensures time reversal symmetry; $U_{m,n}(\sigma)$ and its inverse $U_{m,n}(\sigma)^*$ should have the same probabilities. This condition also ensures that the operator $\mathcal{Q}_{m,n}$ defined in (2.4) is self-adjoint on the Hilbert space $\widehat{\mathcal{B}}(\mathcal{H}_N)$ consisting of $\mathcal{B}(\mathcal{H}_N)$ equipped with the Hilbert–Schmidt inner product $\langle A, B\rangle := \mathrm{Tr}[A^*B]$. Note that the normalized Haar measure has this property. For more discussion, see [9]. This brings us to the following definitions from [9].

Definition 2.1. Define the operators $\mathcal{Q}_N$ and $\mathcal{L}_N$ on $\mathcal{B}(\mathcal{H}_N)$ by

$$\mathcal{Q}_N = \binom{N}{2}^{-1} \sum_{m<n} \mathcal{Q}_{m,n} \quad \text{and} \quad \mathcal{L}_N = N(\mathcal{Q}_N - \mathbb{1}_{\mathcal{H}_N}). \tag{2.5}$$

Definition 2.2 (Quantum Kac Master Equation (QKME)). The *Quantum Kac Master Equation* is the evolution equation on $\mathfrak{S}(\mathcal{H}_N)$ given by

$$\frac{\mathrm{d}}{\mathrm{d}t}\varrho(t) = \mathcal{L}_N\varrho(t).$$

The QKME is solved by exponentiation: for each $t \geq 0$, we may define an operator $\mathcal{P}_{N,t}$ on each $\mathcal{B}(\mathcal{H}_N)$ by

$$\mathcal{P}_{N,t}A = \sum_{k=1}^{\infty} e^{-Nt}\frac{(Nt)^k}{k!}\mathcal{Q}_N^k A = e^{t\mathcal{L}_N}A.$$

Then, the unique solution $\varrho(t)$ of the QKME satisfying $\varrho(0) = \varrho_0 \in \mathfrak{S}(\mathcal{H}_N)$ is

$$\varrho(t) = \mathcal{P}_{N,t}\varrho_0.$$

The operators $\mathcal{Q}_{m,m}$ defined in (2.4) are *completely positive* as are all linear combinations of operators of the form $X \mapsto VXV^*$ for $X, V \in \mathcal{B}(\mathcal{K})$, $\mathcal{K}$ a Hilbert space. Conversely, by theorems of Kraus and Choi [10, 22], every completely positive operator Φ on $\mathcal{K}$, $\mathcal{K}$ a Hilbert space of finite dimension d, has the from

$$\Phi(X) = \sum_{j=1}^{n} V_j X V_j^*,$$

where $n \leq d^2$. The reader unfamiliar with complete positivity may take this as the definition for present purposes.

It follows that the semigroup $\{\mathcal{P}_t\}_{t\geq 0}$ is a semigroup of completely positive operators, and moreover, each $\mathcal{P}_t$ is *unital*, meaning that $\mathcal{P}_t\mathbb{1} = \mathbb{1}$, where $\mathbb{1}$ is the identity in $\mathcal{B}(\mathcal{H}_N)$. Such semigroups are called *quantum Markov semigroups*, and they arise also in the quantum theory of open systems [11] for somewhat different reasons, and there is an extensive literature on them. In particular, there is a structure theorem due to Lindblad [23] and independently to Gorini, Kossakowski, and Sudershan [18] that gives a canonical form for the generator. They proved that generator $\mathcal{L}$ of a quantum Markov semigroup always has the form

$$\mathcal{L}X = i[H, X] + \sum_{j=1}^{n}\left(L_j X L_j^* - \frac{1}{2}L_j L_j^* X - \frac{1}{2}X L_j L_j^*\right)$$

for some self-adjoint operator H on $\mathcal{K}$ (which will be zero in our case) and some finite set $\{L_1, \ldots, L_n\}$ of operators on $\mathcal{K}$. To write our generator in this form, let

$$\mathcal{Q}_N(X) = \sum_{j=1}^{n} V_j X V_j^* \tag{2.6}$$

be a Kraus representation of $\mathcal{Q}_N$. Then, since $\mathcal{Q}_N(\mathbb{1}) = \mathbb{1}$, $\sum_{j=1}^n V_j V_j^* = \mathbb{1}$. Therefore,

$$\mathcal{L}_N X = N \sum_{j=1}^n \left(V_j X V_j^* - \frac{1}{2} V_j V_j^* X - \frac{1}{2} X V_j V_j^* \right). \tag{2.7}$$

Because $\mathcal{Q}_N$ is self-adjoint on $\widehat{\mathcal{B}}(\mathcal{H}_N)$, we also have $\mathcal{Q}_N(X) = \sum_{j=1}^n V_j^* X V_j$, and hence, we may arrange that $\{V_1, \dots, V_n\} = \{V_1^*, \dots, V_n^*\}$. Then, $\mathcal{L}_N$ can be written in terms of commutators as

$$\mathcal{L}_N = \frac{N}{2} \sum_{j=1}^n [V_j^*, [V_j, X]]. \tag{2.8}$$

The operation $X \mapsto [V, X]$ is a derivation on $\mathcal{B}(\mathcal{H}_N)$, and hence, (2.8) displays $\mathcal{L}_N$ as a sort on non-commutative Laplace operator since $X \mapsto [V_j, X]$ is a derivation on $\mathcal{B}(\mathcal{H}_N)$.

We will investigate the spectral gap of $\mathcal{L}_N$ (the least non-zero eigenvalue of $-\mathcal{L}_N$), and in fact, we will determine it exactly. This involves relating the spectrum of $\mathcal{L}_N$ to the spectra of the graph Laplacians $\Delta_{\mathcal{G}_M}$ on a family of graphs $\mathcal{G}_M$, $M \in \mathbb{N}$, associated to the Kac model. In the next section, we explain the quantum dynamical origin of these graphs. The connection between the spectrum of $\mathcal{L}_N$ and the spectra of $\Delta_{\mathcal{G}_M}$, $M \in \mathbb{N}$, will emerge when we rewrite the generator in the form (2.7) or (2.8). The key to this will be to replace the formula (2.5) with Kraus representation (2.6) of $\mathcal{Q}_N$.

3. Discrete structures associated to the quantum Kac model

3.1. The collision graph

To obtain a more detailed picture of the dynamics, we start from the N particle Hamiltonian H_N and the single particle Hamiltonian h out of which it is constructed. Suppose that H is a d-dimensional Hilbert space and h has d eigenvalues $e_1, \dots, e_d$. Let $\{\psi_1, \dots, \psi_d\}$ be an orthonormal basis for $\mathcal{H}$ with $h\psi_j = e_j \psi_j$ for all $1 \le j \le d$.

The eigenvalues of H_N are indexed by the multi-indices $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_N) \in \{1, \dots, d\}^N$ and are given by

$$e(\boldsymbol{\alpha}) = e_{\alpha_1} + \cdots + e_{\alpha_N}. \tag{3.1}$$

We introduce the notation $\mathcal{V}_N$ for the set $\{1, \dots, d\}^N$ of multi-indices because soon it will be the set of vertices on a graph. Defining

$$\Psi_{\boldsymbol{\alpha}} := \psi_{\alpha_1} \otimes \cdots \otimes \psi_{\alpha_N},$$

$\{\Psi_{\boldsymbol{\alpha}} : \boldsymbol{\alpha} \in \mathcal{V}_N\}$ is an orthonormal basis of $\mathcal{H}_N$ consisting of eigenvectors of H_N. For a multi-index $\boldsymbol{\alpha}$ and $k \in \{1, \ldots, d\}$, define the "occupation numbers"

$$\mathbf{k}(\boldsymbol{\alpha}) = (k_1(\boldsymbol{\alpha}), \ldots, k_d(\boldsymbol{\alpha})), \quad k_j(\boldsymbol{\alpha}) = |\{1 \leq m \leq N : \alpha_m = j\}|,$$

where, for a set A, $|A|$ denotes the cardinality of A. Thus, an alternate to the formula (3.1) for $e(\boldsymbol{\alpha})$ is

$$e(\boldsymbol{\alpha}) = \sum_{j=1}^{d} k_j(\boldsymbol{\alpha}) e_j.$$

We also define, for all $1 \leq m < n \leq N$,

$$e_{m,n}(\boldsymbol{\alpha}) = e_{\alpha_m} + e_{\alpha_m}.$$

The quantum dynamics specified by the QKME induces a non-oriented graph structure on $\mathcal{V}_N$

Definition 3.1. For $\boldsymbol{\alpha} \in \mathcal{V}_N$, let $P_{\boldsymbol{\alpha}}$ denote the orthogonal projection onto the span of $\Psi_{\boldsymbol{\alpha}}$. Two vertices $\boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathcal{V}_N$ are *adjacent* in case $\boldsymbol{\alpha} \neq \boldsymbol{\beta}$:

$$\mathrm{Tr}[P_{\boldsymbol{\alpha}} \mathcal{Q}_N(P_{\boldsymbol{\beta}})] > 0, \tag{3.2}$$

Since $\mathcal{Q}_N$ is self-adjoint, $\mathrm{Tr}[P_{\boldsymbol{\alpha}} \mathcal{Q}_N(P_{\boldsymbol{\beta}})] = \mathrm{Tr}[P_{\boldsymbol{\beta}} \mathcal{Q}_N(P_{\boldsymbol{\alpha}})]$, and the adjacency relation is symmetric in $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$. Any such pair of adjacent vertices defines an edge, and we denote the set of all edges by $\mathcal{E}_N$. If $\boldsymbol{\gamma}$ is adjacent to $\boldsymbol{\delta}$, we write $[\boldsymbol{\gamma}, \boldsymbol{\delta}]$ to denote the corresponding edge. Note that $[\boldsymbol{\gamma}, \boldsymbol{\delta}] = [\boldsymbol{\delta}, \boldsymbol{\gamma}]$. We denote this graph by $\mathcal{G}_N$.

The following lemma simplifies the description of adjacency, and its proof explains the origins of the definition.

Lemma 3.2. *Two vertices $\boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathcal{V}_N$ are adjacent if and only if, for some $1 \leq m < n \leq N$,*

$$\beta_p = \alpha_p \quad \textit{for } p \neq m, n, \tag{3.3}$$

and

$$e_{m,n}(\boldsymbol{\alpha}) = e_{m,n}(\boldsymbol{\beta}), \tag{3.4}$$

Proof. Using a common mathematical physics notation for $P_{\boldsymbol{\alpha}}$ and $P_{\boldsymbol{\beta}}$, one can write (3.2) as

$$\langle \Psi_{\boldsymbol{\alpha}}, \mathcal{Q}_N(|\Psi_{\boldsymbol{\beta}}\rangle\langle\Psi_{\boldsymbol{\beta}}|)\Psi_{\boldsymbol{\alpha}}\rangle > 0. \tag{3.5}$$

By (2.4) and (2.5), this is the case if and only if, for some $1 \leq m < n \leq N$ and some $\sigma \in \mathcal{C}$,

$$|\langle \Psi_{\boldsymbol{\beta}}, U_{m,n}(\sigma)\Psi_{\boldsymbol{\alpha}}\rangle|^2 > 0. \tag{3.6}$$

Since $U_{m,n}(\sigma)$ acts non-trivially only on factors m and n of $\mathscr{H}_N$, (3.6) is possible only in case (3.3) is satisfied. Moreover, since $U_{m,n}(\sigma)$ commutes with H_N so that the collisions conserve energy, (3.6) is possible only in case (3.4) is satisfied.

On the other hand, if (3.3) and (3.4) are satisfied, there will be some $U(\sigma) \in \mathcal{C}$ such that (3.6) is satisfied. Then, when the probability measure ν has a strictly positive density with respect to normalized Haar measure on $\mathcal{C}$, (3.5) is satisfied since $\sigma \mapsto |\langle \Psi_{\boldsymbol{\beta}}, U_{m,n}(\sigma)\Psi_{\boldsymbol{\alpha}}\rangle|^2$ is continuous. ∎

It is evident that if $[\boldsymbol{\gamma}, \boldsymbol{\delta}] \in \mathscr{E}_N$, then $e(\boldsymbol{\gamma}) = e(\boldsymbol{\delta})$, but the converse need not be true, even when the probability measure ν on $\mathcal{C}$ is normalized Haar measure. However, as we now explain, a simple non-degeneracy condition on the spectrum of H_2 will guarantee this.

Definition 3.3. The spectrum of h is *strongly non-degenerate* when the following two conditions are satisfied.

(1) The spectrum of h is such that the spectrum of H_2 is non-degenerate on the symmetric subspace of $\mathscr{H}_2 = \mathscr{H} \otimes \mathscr{H}$. That is, for any $1 \leq j_1, j_2, j_3, j_4 \leq d$,

$$e_{j_1} + e_{j_2} = e_{j_3} + e_{j_4} \iff \{j_1, j_2\} = \{j_3, j_4\}. \tag{3.7}$$

(2) For each $N \geq 3$ and each $E \in \sigma(H_N)$, the pair of equations

$$\sum_{m=1}^{d} k_m e_n = E \quad \text{and} \quad \sum_{m=1}^{d} k_m = N \tag{3.8}$$

has exactly one solution for each E in the spectrum of $\mathscr{H}_N$.

Note that when (3.7) is satisfied, the spectrum of h is necessarily non-degenerate. The condition (3.7) has the consequence that if $[\boldsymbol{\gamma}, \boldsymbol{\delta}] \in \mathscr{E}_N$, then $\boldsymbol{\gamma}$ and $\boldsymbol{\delta}$ differ by a pair transposition. In particular, $\mathbf{k}(\boldsymbol{\gamma}) = \mathbf{k}(\boldsymbol{\delta})$, and thus, under condition (3.7), both the occupation number function $\mathbf{k}$ and the energy e are constant on every connected component of $\mathscr{G}_N$.

The further condition (3.8) ensures that if $e(\boldsymbol{\gamma}) = e(\boldsymbol{\delta})$, then $\boldsymbol{\gamma}$ and $\boldsymbol{\delta}$ belong to the same connected component of $\mathscr{G}_N$. Suppose that the pair of equations (3.8) has exactly one solution for each E in the spectrum of $\mathscr{H}_N$. Then, $e(\boldsymbol{\gamma}) = e(\boldsymbol{\delta})$ if and only if $\mathbf{k}(\boldsymbol{\gamma}) = \mathbf{k}(\boldsymbol{\delta})$, which in turn is the case if and only if $\boldsymbol{\gamma}$ and $\boldsymbol{\delta}$ are related by a finite sequence of pair transpositions. Then, $[\boldsymbol{\gamma}, \boldsymbol{\delta}] \in \mathscr{E}_N$ if and only if $\boldsymbol{\gamma}$ and $\boldsymbol{\delta}$ differ by a pair transposition. That is, under conditions (3.7) and (3.8), the eigenspaces $\mathscr{H}_E$ of H_N may be identified with the connected components of the graph $\mathscr{G}_N$.

When $\{e_1, \ldots, e_d\}$ is linearly independent over the rationals, both conditions (3.7) and (3.8) are evidently satisfied. Moreover, (3.7) does not imply (3.8).

Example 3.4. Assume that the single-particle Hamiltonian has the eigenvalues $1, 2, 4$, each with multiplicity one. Then, (3.7) is satisfied: H_2 has the 6 eigenvalues 2, 3, 4, 5, 6, and 8 on $\mathcal{H} \otimes_{\mathrm{sym}} \mathcal{H}$. However, (3.8) is not always satisfied. To see this, let $N \geq 9$ so that there are at least two positive even integers n_1 such that $2n_1 \leq N$. Pick such an n_1 and then define

$$n_2 := N - \frac{3}{2}n_1, \quad n_3 := \frac{1}{2}n_1.$$

Then,

$$n_1 + 2n_2 + 4n_3 = 2N \quad \text{and} \quad n_1 + n_2 + n_3 = N.$$

The number $e = 2N$ is an eigenvalue of the Hamiltonian H_N, but there are $\boldsymbol{\gamma}, \boldsymbol{\delta} \in \mathcal{V}_3$ such that $\mathbf{k}(\boldsymbol{\gamma}) \neq \mathbf{k}(\boldsymbol{\delta})$. For example, take $N = 9$. Then, the construction above yields $\boldsymbol{\gamma}, \boldsymbol{\delta} \in \mathcal{V}_3$ such that $e(\boldsymbol{\gamma}) = e(\boldsymbol{\delta}) = 18$, but $k_1(\boldsymbol{\delta}) = 2$ and $k_1(\boldsymbol{\gamma}) = 4$. In such examples, there are eigenvalues of H_N such that the corresponding eigenspaces are spanned by vectors Ψ_α belonging to different connected components of $\mathcal{G}_N$.

In summary, under conditions (3.7) and (3.8), $\boldsymbol{\gamma}$ and $\boldsymbol{\delta}$ are adjacent if and only if they differ by a pair transpositions, and the connected components of $\mathcal{G}_N$ are indexed by the eigenvalues E of H_N. For $E \in \mathrm{Spec}(H_N)$, write $\mathcal{G}_{N,E}$ to denote the connected component of $\mathcal{G}_N$ on which $e(\boldsymbol{\gamma}) = E$ for all $\boldsymbol{\gamma}$ in its vertex set, $\mathcal{V}_{M,E}$.

Let $\mathbf{k}$ be the occupation vector given by the unique solution of (3.8) for N and E. Then, evidently the cardinality of $\mathcal{V}_{N,E}$ is

$$d_{\mathbf{k}} := \frac{N!}{k_1! \cdots k_d!}.$$

For each $\boldsymbol{\alpha} \in \mathcal{V}_N$, let $v(\boldsymbol{\alpha})$ denote the *valency* of $\boldsymbol{\alpha}$, i.e., the number of vertices in $\mathcal{G}_N$ that are adjacent to $\boldsymbol{\alpha}$.

Assume strong non-degeneracy. For each $\boldsymbol{\alpha}$, there are either one or zero vertices that are adjacent to $\boldsymbol{\alpha}$ through collision involving particles m and n according to whether α_m and α_n are distinct or not. Summing over $m < n$, the valency of $\boldsymbol{\alpha}$ is given by

$$v(\boldsymbol{\alpha}) = \sum_{m<n} D(1 - \delta_{\alpha_m,\alpha_n}) = \sum_{i<j}^{d} k_i(\boldsymbol{\alpha})k_j(\boldsymbol{\alpha}).$$

Hence, under the assumption of strong non-degeneracy, $\mathcal{G}_N$ is a regular graph.

3.2. The graph Laplacian

Given a finite undirected graph $\mathcal{G}$ with vertex set $\mathcal{V}$ and edge set $\mathcal{E}$, the *graph Laplacian* $\Delta_{\mathcal{G}}$ is the operator on functions f on $\mathcal{V}$ given by

$$\Delta_{\mathcal{G}} f(x) = \sum_{y \in \mathcal{V}:\{x,y\} \in \mathcal{E}} (f(x) - f(y)).$$

Note that

$$\sum_{x\in\mathcal{V}} f(x)\Delta_{\mathcal{G}} f(x) = \sum_{y\in\mathcal{V}:\{x,y\}\in\mathcal{E}} \frac{1}{2}(f(x)-f(y))^2. \tag{3.9}$$

This computation shows that if $\mu_{\mathcal{V}}$ denotes the uniform probability measure on $\mathcal{V}$, $L_{\mathcal{G}}$ is a positive semi-definite operator on $L^2(\mu_{\mathcal{V}})$, and that the constant function $f(x) = 1$ for all $x \in \mathcal{V}$ is an eigenfunction with eigenvalue 0. (This is the standard sign convention for the Laplacian in graph theory.)

It follows from (3.9) that $\Delta_{\mathcal{G}} f = 0$ if and only if f is constant on each connected component of $\mathcal{G}$. Hence, on a connected graph $\mathcal{G}$, 0 is an eigenvalue of multiplicity one, and the eigenspace is spanned by the constant vector. The quadratic form on the right in (3.9) is called the *Dirichlet form* of the graph Laplacian.

One of the main results of this paper is that there is a very close connection between the spectrum of $\Delta_{\mathcal{G}_N}$ and the spectrum of $\mathcal{L}_N$. In fact, if one knows the full spectrum of $\Delta_{\mathcal{G}_N}$ for every N, then Theorem 5.3 proved below yields the full spectrum of $-\mathcal{L}_N$ for all N under the assumption that the spectrum of h is strongly non-degenerate, and the collision law ν is the uniform Haar measure on $\mathcal{C}$.

Definition 3.5. Let $\mathcal{G}$ be a finite connected graph with vertex set $\mathcal{V}$. The *spectral gap* of $\mathcal{G}$, $\Gamma_{\mathcal{G}}$, is the least non-zero eigenvalue of $\Delta_{\mathcal{G}}$.

By the Rayleigh–Ritz variational principle,

$$\Gamma_{\mathcal{G}} = \inf\left\{\int_{\mathcal{V}} f(x)\Delta_{\mathcal{G}} f(x)\mathrm{d}\mu_{\mathcal{V}} : \int_{\mathcal{V}} f(x)\mathrm{d}\mu_{\mathcal{V}} = 0,\ \int_{\mathcal{V}} |f(x)|^2\mathrm{d}\mu_{\mathcal{V}} = 1\right\}.$$

3.3. Equilibrium states

The set of equilibrium states for the QKME is considerably richer than for the classical Kac model. We present here a summary of some relevant results obtained in [9].

A density matrix ϱ on $\mathcal{H}_N$ is an *equilibrium state* if and only if $\mathcal{L}_N\varrho = 0$ so that $\mathcal{P}_t\varrho = \varrho$ for all $t > 0$. By Definition 2.1,

$$\mathcal{L}_N\varrho = 0 \iff \mathcal{Q}_N(\varrho) = \varrho.$$

Thus, the problem of identifying all equilibrium states is the problems of identifying all fixed-point states under the completely positive, unital, and self-adjoint operator $\mathcal{Q}_N$.

For the classical Kac model, thought of in terms of a stochastic process on $\mathbb{R}^N$, the equilibrium states are precisely the probability densities ϱ on $\mathbb{R}^N$ that are functions of the energy $\frac{1}{2}\sum_{j=1}^N v_j^2$. This is because any function on $\mathbb{R}^N$ that is invariant under all planar rotations is constant on each level-surface of the energy due to the fact that averaging a function over all planar rotations has the same effect as averaging the function over all rotations.

In the quantum setting, things are somewhat more complicated. Consider an N particle quantum Kac model in which the collision law ν is normalized Haar measure.

Let $E \in \mathrm{Spec}(H_N)$, the spectrum of H_N, and let $\mathcal{K}_{N,E}$ denote corresponding eigenspace. Let $P_{N,E}$ denote the orthogonal projection onto $\mathcal{K}_{N,E}$. Then,

$$\mathcal{H}_N = \bigoplus_{E \in \mathrm{Spec}(H_N)} \mathcal{K}_{N,E}.$$

The Hilbert spaces $\mathcal{K}_{N,E}$ are the analogs of the energy shells $\mathcal{S}_{N,E}$ in the classical Kac model. Define the density matrix ϱ_E by

$$\varrho_{N,E} := \frac{1}{\dim(\mathcal{K}_E)} P_{N,E}.$$

This is the direct analog of the uniform probability measure on $\mathcal{S}_{N,E}$ in the classical Kac model. Then, each $\varrho_{N,E}$ is an equilibrium state for the Kac model. That is, for all E,

$$\mathcal{Q}_N(\varrho_{N,E}) = \varrho_{N,E},$$

which is true because each $\varrho_{N,E}$ is a polynomial in H_N, and hence, $\varrho_{N,E}$ commutes with every $U_{m,n}(\sigma)$, $\sigma \in \mathcal{C}$.

However, as explained in [9], at this level of generality, it may be that $P_{N,E}$ can be decomposed as the sum of two (or more) non-trivial orthogonal projections

$$P_{N,E} = P + Q$$

satisfying $\mathcal{Q}_N(P) = P$ and $\mathcal{Q}(Q) = Q$. Then, $\frac{1}{\mathrm{Tr}[P]} P$ and $\frac{1}{\mathrm{Tr}[Q]} Q$ are equilibrium states, and they are not normalized projections onto energy eigenspaces. This is exactly what happens in Example 3.4. We can decide whether or not this happens based on the structure of the graph $\mathcal{G}_N$.

The following result is proved in [9], although it is stated in somewhat different terms, not explicitly mentioning the graph $\mathcal{G}_N$, but using the same notion of "connected component".

Theorem 3.6. *The set density matrices $\varrho \in \mathcal{B}(\mathcal{H}_N)$ satisfying $\mathcal{Q}_N(\varrho) = \varrho$ is precisely convex hull of the set*

$$\{\varrho_{N,E} : E \in \mathrm{spec}(H_N)\} \tag{3.10}$$

if and only if all $\boldsymbol{\gamma}$ and $\boldsymbol{\delta}$ such that $e(\boldsymbol{\gamma}) = e(\boldsymbol{\delta})$ belong to the same connected component of $\mathcal{G}_N$.

As we have seen above, if we make the assumption that the spectrum of h is strongly non-degenerate (in addition to the assumption that ν is normalized Haar measure), then all $\boldsymbol{\gamma}$ and $\boldsymbol{\delta}$ such that $e(\boldsymbol{\gamma}) = e(\boldsymbol{\delta})$ do belong to the same connected

component of $\mathcal{G}_N$. Thus, under this condition, the set of equilibrium states is precisely the convex hull of the set in (3.10). *For the rest of this paper, we assume that the spectrum of h is strongly non-degenerate.*

Write $\mathcal{B}(\mathcal{K}_{N,E})$ to denote the subalgebra $P_{N,E}\mathcal{B}(\mathcal{H}_N)P_{N,E}$ consisting of operators on $\mathcal{B}(\mathcal{H}_N)$ that act non-trivially only on $\mathcal{K}_{N,E}$. Because $P_{N,E}$, being a function of H_N, commutes with every unitary that commutes with H_N, for all $X \in \mathcal{B}(\mathcal{H}_N)$,

$$P_{N,E}\mathcal{Q}_N(X)P_{N,E} = \mathcal{Q}_N(P_{N,E}XP_{N,E}).$$

It follows that each $\mathcal{B}(\mathcal{K}_{N,E})$ is invariant under $\mathcal{P}_{N,t}$ for each $t > 0$, and the generator $\mathcal{L}_N$. Define

$$\mathcal{L}_{N,E} := \mathcal{L}_N\big|_{\mathcal{B}(\mathcal{K}_{N,E})}.$$

In this finite-dimensional setting, it is easy to show that, for any density matrix $\varrho \in \mathcal{B}(\mathcal{K}_{N,E})$, $\lim_{t\to\infty}\mathcal{P}_t\varrho$ exists and is an equilibrium state in $\mathcal{B}(\mathcal{K}_{N,E})$. Since there is exactly one equilibrium state in $\mathcal{B}(\mathcal{K}_{N,E})$, namely, $\varrho_{N,E}$,

$$\lim_{t\to\infty}\mathcal{P}_t\varrho = \varrho_{N,E}, \tag{3.11}$$

as shown in [9]. This is the analog of the convergence to the uniform distribution on each $\mathcal{S}_{N,E}$ in the classical Kac model.

3.4. Main results and methods

Let ϱ be a density matrix in $\mathcal{B}(\mathcal{K}_{N,E})$. In this paper, we are concerned with determining the rate of convergence in (3.11) in terms of the *spectral gap*, $\Gamma_{\mathcal{L}_{N,E}}$, for the generator $\mathcal{L}_{N,E}$ of the QKME on $\mathcal{B}(\mathcal{K}_{N,E})$. Since the nullspace of $\mathcal{L}_N$ restricted to $\mathcal{B}(\mathcal{K}_{N,E})$ is spanned by $\varrho_{N,E}$, this spectral gap is the smallest positive eigenvalue of $-\mathcal{L}_N$ restricted to $\mathcal{B}(\mathcal{K}_{N,E})$. We will prove the following theorem.

Theorem 3.7. *Consider a quantum Kac model based on a single-particle Hamiltonian h whose spectrum is strongly non-degenerate, and in which the collision measure ν is the normalized Haar measure on the collision group $\mathcal{C}$. Then, for all $N \geq 2$, all $d \geq 2$, and all $E \in \mathrm{Spec}(H_N)$ such that $\dim(\mathcal{K}_{N,E}) > 1$, the spectral gap of $\mathcal{L}_{N,E}$, $\Gamma_{\mathcal{L}_{N,E}}$ is given by*

$$\Gamma_{\mathcal{L}_{N,E}} = \frac{N}{N-1}.$$

As a consequence of Theorem 3.7 and the spectral theorem, for any $X \in \mathcal{B}(\mathcal{K}_{N,E})$ such that $\mathrm{Tr}[\varrho_E X] = 0$,

$$\|\mathcal{P}_t(X)\|_2 \leq e^{-t\frac{N}{N-1}}\|X\|_2,$$

where $\|\cdot\|_2$ denotes the Hilbert–Schmidt norm on $\mathcal{B}(\mathcal{K}_{N,E})$. The fact that this rate of equilibration does not decrease to zero as N increases to infinity is significant for the applications developed in [9]. (Note that if $\dim(\mathcal{K}_{N,E}) = 1$ and $X \in \mathcal{B}(\mathcal{K}_{N,E})$, $\mathrm{Tr}[X] = 0$ implies $X = 0$.)

In this paper, we focus on the graph theoretical results that are basic to the proof of Theorem 3.7. As we have already seen in Theorem 3.6, there is a close connection between the generator $\mathcal{L}_N$ and the graph $\mathcal{G}_N$. In Theorem 5.3, we prove a formula that expresses the entire spectrum of $\mathcal{L}_N$ in terms of the spectrum of $\Delta_{\mathcal{G}_M}$ for all $M \leq N$.

Once this is in hand, the remaining problem is to determine the spectrum of $\Delta_{\mathcal{G}_M}$ for all M. Under our conditions on the Kac model, $\mathcal{G}_N$ turns out to be a graph known as the *multislice*, and the full spectrum of the graph Laplacian for the multislice is known. However, for the purpose of proving Theorem 3.7, we need much less than knowledge of the full spectrum of $\Delta_{\mathcal{G}_M}$ for all M.

In fact, the ideas we have developed for determining the spectral gap in the classical Kac model [6, 8, 9] are relevant to determining the spectral gap of $\Delta_{\mathcal{G}_M}$ for all M, and we develop this approach here. The approach is quite robust, and we expect it be applicable to a range of problems that will arise when other collision models are investigated in which the graphs are more complicated and the edges are weighted.

4. The Lindblad form of the QKME

When the collision law ν is normalized Haar measure, the operators Ω_{mn} specified in (2.4) are not only self-adjoint; they are orthogonal projections since, due to the invariance properties of Haar measure,

$$U_{mn}(\sigma)\Omega_{mn}U_{mn}^*(\sigma) = \Omega_{mn}$$

for all σ and hence $\Omega_{mn}^2 = \Omega_{mn}$. It is easy to pass from an explicit form of these projections to the Lindblad form of the QKME.

Consider first the case $N = 2$. The subalgebra $\mathcal{M}$ of $\mathcal{B}(\mathcal{H}_2)$ consisting of functions of H_2 is a von Neumann subalgebra of $\mathcal{B}(\mathcal{H})$, as is its commutant $\mathcal{M}'$. Any von Neumann algebra is spanned by the unitaries it contains, and hence, $\mathcal{M}'$ is spanned by the unitaries that commute with H_2, which is, by definition, $\mathcal{C}$. By von Neumann's double commutant theorem,

$$\mathcal{M} = \mathcal{M}'' = \mathcal{C}'.$$

Evidently, the range of the projection Ω_{12} is precisely $\mathcal{C}' = \mathcal{M}$. Therefore, if

$$H_2 = \sum_{E \in \Sigma_2} E P_E$$

is the spectral decomposition of H_2,

$$\mathcal{Q}_{12}(X) = \sum_{E\in\Sigma_2} \frac{1}{D(E)} \mathrm{Tr}[XP_E]P_E, \tag{4.1}$$

where

$$D(E) = \mathrm{Tr}[P_E]$$

is the degeneracy of the eigenvalue E. From here, it is easy to write down a Kraus representation of $\mathcal{Q}_{12}$ in terms of the orthonormal basis $\{\psi_{\alpha_1}\otimes\psi_{\alpha_2} : 1 \le \alpha_1, \alpha_2 \le d\}$ of $\mathcal{H}_2$. Since

$$\mathrm{Tr}[XP_E] = \sum_{e_{\alpha_1}+e_{\alpha_2}=E} \langle \psi_{\alpha_1}\otimes\psi_{\alpha_2}, X\psi_{\alpha_1}\otimes\psi_{\alpha_2}\rangle$$

and

$$P_E := \sum_{e_{\beta_1}+e_{\beta_2}=E} |\psi_{\beta_1}\otimes\psi_{\beta_2}\rangle\langle\psi_{\beta_1}\otimes\psi_{\beta_2}|,$$

if we define

$$F_{\alpha_1\alpha_2;\beta_1\beta_2} := |\psi_{\alpha_1}\otimes\psi_{\alpha_2}\rangle\langle\psi_{\beta_1}\otimes\psi_{\beta_2}|,$$

then

$$\mathcal{Q}_{12}(X) = \sum_{E\in\Sigma_2} \frac{1}{D(E)} \Big(\sum_{e_{\alpha_1}+e_{\alpha_2}=e_{\beta_1}+e_{\beta_2}=E} F^*_{\alpha_1\alpha_2;\beta_1\beta_2} X F_{\alpha_1\alpha_2;\beta_1\beta_2} \Big).$$

Evidently, $\mathcal{Q}_{N,m,n}$ is completely positive. Since Haar measure on $\mathcal{U}$ is invariant under the map $U \mapsto U^*$, $\mathcal{Q}_{N,m,n}$ is self-adjoint with respect to the Hilbert–Schmidt inner product on $\mathcal{B}(\mathcal{H}_N)$. It is evidently unital and trace preserving.

We now lift $\mathcal{Q}_{12}$ to $\mathcal{H}_N$ as described in the beginning of this section by fixing $1 \le m < n \le N$ and replacing each U by $U_{m,n}$, and thus obtaining $\mathcal{Q}_{m,n}$, which now describes the averaged effect of a collision between particles m and n. For every $1 \le m < n \le N$, $\mathcal{Q}_{m,n}$ is completely positive, self-adjoint with respect to the Hilbert–Schmidt inner product on $\mathcal{B}(\mathcal{H}_N)$, unital, and trace preserving because it inherits these properties from $\mathcal{Q}_{12}$.

In lifting $\mathcal{Q}$ up to $\mathcal{H}_N$ as described, the trace in (4.1) becomes the partial trace over the mth and nth factors in $\mathcal{H}_N$. For $(m,n) = (1,2)$, one easily finds

$$\mathcal{Q}_{1,2}(X) = \sum_{\alpha_1,\alpha_2,\beta_1,\beta_2; e_{\alpha_1}+e_{\alpha_2}=e_{\beta_1}+e_{\beta_2}} \frac{1}{D(e_{\alpha_1}+e_{\alpha_2})} E^*_{\alpha_1\alpha_2;\beta_1\beta_2} X E_{\alpha_1\alpha_2;\beta_1\beta_2},$$

where

$$\begin{aligned} E_{\alpha_1\alpha_2;\beta_1\beta_2} &= |\psi_{\alpha_1}\otimes\psi_{\alpha_2}\rangle\langle\psi_{\beta_1}\otimes\psi_{\beta_2}| \otimes \mathbb{1}_{N-2} \\ &= |\psi_{\alpha_1}\rangle\langle\psi_{\beta_1}| \otimes |\psi_{\alpha_2}\rangle\langle\psi_{\beta_2}| \otimes \mathbb{1}_{N-2}, \end{aligned}$$

and $\mathbb{1}_{N-2}$ is the identity operator on the remaining factor. For general $m < n$, the rank one operators $|\psi_{\alpha_1}\rangle\langle\psi_{\beta_1}|$ and $|\psi_{\alpha_2}\rangle\langle\psi_{\beta_2}|$ should be inserted as factors m, respectively, n in the tensor product and the remaining factors are the identity matrices. Therefore, for $1 \le m < n \le N$,

$$\mathcal{Q}_{m,n}(X) = \sum_{\alpha_m,\alpha_n,\beta_m,\beta_n;e_{\alpha_m}+e_{\alpha_n}=e_{\beta_m}+e_{\beta_n}} \frac{1}{D(e_{\alpha_m}+!e_{\alpha_n})} E^*_{\alpha_m\alpha_n;\beta_m\beta_n} X E_{\alpha_m\alpha_n;\beta_m\beta_n}, \tag{4.2}$$

where

$$E_{\alpha_m\alpha_n;\beta_m\beta_n} = |\psi_{\alpha_m}\rangle\langle\psi_{\beta_m}| \otimes |\psi_{\alpha_n}\rangle\langle\psi_{\beta_n}| \otimes \mathbb{1}_{N-2},$$

with the subscripts indicating the factors on which the first two terms operate. Finally, define

$$\mathcal{Q}(X) = \binom{N}{2}^{-1} \sum_{m<n} \mathcal{Q}_{mn}(X).$$

Note that (4.2) gives the Kraus form [22] of the completely positive operator $\mathcal{Q}_{m,n}$, and then summing, we have the Kraus form of $\mathcal{Q}$. From this, one can easily write down the Lindblad form [23] of the generator $\mathcal{L}_N$, but here it turns out to be more convenient to work directly with (4.2).

To make use of (4.2), we introduce a natural orthonormal basis for $\mathcal{B}(\mathcal{H}_N)$: for $\boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathcal{V}_N$, define

$$F_{\boldsymbol{\alpha}\boldsymbol{\beta}} := |\Psi_{\boldsymbol{\alpha}}\rangle\langle\Psi_{\boldsymbol{\beta}}|.$$

Since $\{\Psi_{\boldsymbol{\alpha}}\}_{\boldsymbol{\alpha}\in\mathcal{V}_N}$ is an orthonormal basis for $\mathcal{H}_N$, $\{F_{\boldsymbol{\alpha}\boldsymbol{\beta}} : \boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathcal{V}_N\}$ is an orthonormal basis of $\mathcal{B}(\mathcal{H}_N)$.

The operator $\mathcal{Q}$ turns out to have a fairly simple matrix representation in the $\{F_{\boldsymbol{\alpha},\boldsymbol{\beta}}\}$ basis, as we now show. It will be useful to define

$$f_{\alpha\beta} = |\psi_\alpha\rangle\langle\psi_\beta|.$$

We will also make use of the *swap map*, both as a map from $\mathcal{V}_N$ into itself and as a unitary operator on $\mathcal{H}_N$. First, we use a map from $\mathcal{V}_N$ into itself; for $m < n$, and $\boldsymbol{\alpha} \in \mathcal{V}_N$, $S_{mn}(\boldsymbol{\alpha})$ is defined by

$$(S_{mn}(\boldsymbol{\alpha}))_j = \begin{cases} \boldsymbol{\alpha}_n, & j = m, \\ \boldsymbol{\alpha}_m, & j = n, \\ \boldsymbol{\alpha}_j, & j \neq m, n. \end{cases}$$

The *swap operator* is the unitary operator on $\mathcal{H}_N$ defined by

$$S_{mn}\Psi_\alpha = \Psi_{S_{mn}(\boldsymbol{\alpha})}.$$

The following theorem says that $\mathcal{Q}_N(F_{\boldsymbol{\gamma},\boldsymbol{\delta}})$ is a linear combination of the $F_{\boldsymbol{\alpha},\boldsymbol{\beta}}$ in which for some $1 \le m < n \le N$, $\boldsymbol{\alpha} = S_{m,n}\boldsymbol{\gamma}$ and $\boldsymbol{\beta} = S_{m,n}\boldsymbol{\delta}$, and also for this same m and n, $\gamma_m = \delta_m$ and $\gamma_n = \delta_n$. In particular, if

$$D_{\boldsymbol{\gamma},\boldsymbol{\delta}} := \{n : \gamma_n \neq \delta_n\}$$

and $\langle F_{\boldsymbol{\alpha},\boldsymbol{\beta}}, \mathcal{Q}_N(F_{\boldsymbol{\gamma},\boldsymbol{\delta}})\rangle \neq 0$, then $D_{\boldsymbol{\alpha},\boldsymbol{\beta}} = D_{\boldsymbol{\gamma},\boldsymbol{\delta}}$. This provides a large number of invariant subspaces of $\mathcal{Q}_N$ that greatly facilitates the determination of its spectrum, and moreover, it says that the only "active indices" in $\boldsymbol{\gamma}$ and $\boldsymbol{\delta}$ are those in the *complement* of $D_{\boldsymbol{\gamma},\boldsymbol{\delta}}$, and these change on lockstep through pair transpositions. This is the origin on the close link between $\mathcal{L}_N$ and the operators $\Delta_{\mathcal{G}_M}$, where $M \le N$ will correspond to the number of "active indices".

Theorem 4.1. *For all $N \ge 2$ and all $\boldsymbol{\gamma}, \boldsymbol{\delta} \in \mathcal{V}_N$,*

$$\begin{aligned}\binom{N}{2}\mathcal{Q}_N(F_{\boldsymbol{\gamma}\boldsymbol{\delta}}) &= \frac{1}{2}\sum_{m<n} \delta_{\gamma_m\delta_m}\delta_{\gamma_n\delta_n}[F_{\boldsymbol{\gamma}\boldsymbol{\delta}} + S_{mn}F_{\boldsymbol{\gamma}\boldsymbol{\delta}}S_{mn}] \\ &= \frac{1}{2}\sum_{m<n} \delta_{\gamma_m\delta_m}\delta_{\gamma_n\delta_n}[F_{\boldsymbol{\gamma}\boldsymbol{\delta}} + F_{S_{mn}(\boldsymbol{\gamma})S_{mn}(\boldsymbol{\delta})}].\end{aligned}$$

Proof. For simplicity, we pick the pair $(m,n) = (1,2)$. Then,

$$\begin{aligned}&E^*_{\alpha_1\alpha_2;\beta_1\beta_2}F_{\boldsymbol{\gamma}\boldsymbol{\delta}}E_{\alpha_1\alpha_2;\beta_1\beta_2} \\ &\quad= [f_{\beta_1\alpha_1}\otimes f_{\beta_2\alpha_2}\otimes I_{N-2}]\left[\bigotimes_{j=1}^{N} f_{\gamma_j\delta_j}\right][f_{\alpha_1\beta_1}\otimes f_{\alpha_2\beta_2}\otimes I_{N-2}] \\ &\quad= f_{\beta_1\alpha_1}f_{\gamma_1\delta_1}f_{\alpha_1\beta_1}\otimes f_{\beta_2\alpha_2}f_{\gamma_2\delta_2}f_{\alpha_2\beta_2}\bigotimes_{j=3}^{N} f_{\gamma_j\delta_j} \\ &\quad= \delta_{\alpha_1\gamma_1}\delta_{\delta_1\alpha_1}\delta_{\alpha_2\gamma_2}\delta_{\delta_2\alpha_2}f_{\beta_1\beta_1}\otimes f_{\beta_2\beta_2}\bigotimes_{j=3}^{N} f_{\gamma_j\delta_j}.\end{aligned}$$

The sum

$$\sum_{\alpha_1,\alpha_2,\beta_1,\beta_2;e_{\alpha_1}+e_{\alpha_2}=e_{\beta_1}+e_{\beta_2}} \frac{1}{D(e_{\alpha_1}+e_{\alpha_2})}E^*_{\alpha_1\alpha_2;\beta_1\beta_2}F_{\boldsymbol{\gamma}\boldsymbol{\delta}}E_{\alpha_1\alpha_2;\beta_1\beta_2}$$

has a contribution from the non-degenerate eigenvalues of H_2 given by $2e, e \in \sigma(h)$

$$\begin{aligned}E^*_{\alpha_1\alpha_1;\alpha_1\alpha_1}F_{\boldsymbol{\gamma}\boldsymbol{\delta}}E_{\alpha_1\alpha_1;\alpha_1\alpha_1} &= \delta_{\gamma_1\delta_1}\delta_{\gamma_2\delta_2}\delta_{\gamma_1\gamma_2}f_{\gamma_1\gamma_1}\otimes f_{\gamma_1\gamma_1}\bigotimes_{j=3}^{N} f_{\gamma_j\delta_j} \\ &= \delta_{\gamma_1\delta_1}\delta_{\gamma_2\delta_2}\delta_{\gamma_1\gamma_2}F_{\boldsymbol{\gamma}\boldsymbol{\delta}}.\end{aligned}$$

and a contribution from the doubly degenerate eigenvalues of h, $e_i + e_j$, $i \neq j$,

$$\frac{1}{2} \sum_{\alpha_1,\alpha_2,\beta_1,\beta_2;e_{\alpha_1}+e_{\alpha_2}=e_{\beta_1}+e_{\beta_2}} E^*_{\alpha_1\alpha_2;\beta_1\beta_2} F_{\boldsymbol{\gamma\delta}} E_{\alpha_1\alpha_2;\beta_1\beta_2},$$

which for $\gamma_1 \neq \gamma_2$ equals

$$\begin{aligned}
&\frac{\delta_{\gamma_1\delta_1}\delta_{\gamma_2\delta_2}}{2}\left[f_{\gamma_1\gamma_1} \otimes f_{\gamma_2\gamma_2} \bigotimes_{j=3}^{N} f_{\gamma_j\delta_j} + f_{\gamma_2\gamma_2} \otimes f_{\gamma_1\gamma_1} \bigotimes_{j=3}^{N} f_{\gamma_j\delta_j} \right] \\
&= \frac{\delta_{\gamma_1\delta_1}\delta_{\gamma_2\delta_2}}{2}\left[f_{\gamma_1\delta_1} \otimes f_{\gamma_2\delta_2} \bigotimes_{j=3}^{N} f_{\gamma_j\delta_j} + f_{\gamma_2\delta_2} \otimes f_{\gamma_1\delta_1} \bigotimes_{j=3}^{N} f_{\gamma_j\delta_j} \right] \\
&= \frac{\delta_{\gamma_1\delta_1}\delta_{\gamma_2\delta_2}}{2}[F_{\boldsymbol{\gamma\delta}} + S_{12} F_{\boldsymbol{\gamma\delta}} S_{12}].
\end{aligned}$$

Hence, we have

$$\begin{aligned}
\mathcal{Q}_{12}(F_{\boldsymbol{\gamma\delta}}) &= \begin{cases} \delta_{\gamma_1\delta_1}\delta_{\gamma_2\delta_2}\delta_{\gamma_1\gamma_2} F_{\boldsymbol{\gamma\delta}} & \text{if } \gamma_1 = \gamma_2 \\ \frac{\delta_{\gamma_1\delta_1}\delta_{\gamma_2\delta_2}}{2}[F_{\boldsymbol{\gamma\delta}} + S_{12} F_{\boldsymbol{\gamma\delta}} S_{12}] & \text{if } \gamma_1 \neq \gamma_2 \end{cases} \\
&= \frac{\delta_{\gamma_1\delta_1}\delta_{\gamma_2\delta_2}}{2}[F_{\boldsymbol{\gamma\delta}} + S_{12} F_{\boldsymbol{\gamma\delta}} S_{12}]
\end{aligned}$$

since for $\gamma_1 = \gamma_2$ the swap operator S_{12} acts trivially. The same reasoning yields the analogous result for all other $m < n$. Summing and then using (2.5) prove the theorem. ∎

5. The spectrum of the Kac generator $\mathcal{L}_N$

5.1. Direct sum decomposition of $\mathcal{B}(\mathcal{H}_N)$

As explained in the paragraph above Theorem 4.1, this theorem gives rise to a direct sum decomposition of $\mathcal{B}(\mathcal{H}_N)$ into subspaces that are invariant under $\mathcal{L}_N$.

Definition 5.1. For any $\boldsymbol{\delta}, \boldsymbol{\gamma} \in \mathcal{V}_N$, define $C_{\boldsymbol{\delta\gamma}} \subseteq \{1, \ldots, N\}$ to be the *coincidence set* of this pair of vertices. That is,

$$C_{\boldsymbol{\delta\gamma}} = \{j : \delta_j = \gamma_j\}.$$

Next, let $S \subsetneq \{1, \ldots, N\}$.

(1) Define the set of *exterior pair configurations* E_S to be the set of pairs $\boldsymbol{\zeta}, \boldsymbol{\eta} \in \{1, \ldots, d\}^{S^c}$ such that, for all $j \in S^c$, $\zeta_j \neq \eta_j$.

(2) For each $S \subsetneq \{1, \dots, N\}$ and each $(\boldsymbol{\zeta}, \boldsymbol{\eta}) \in E_S$, define $\mathcal{B}_{S;\boldsymbol{\zeta},\boldsymbol{\eta}}$ to be the subspace of $\mathcal{B}(\mathcal{H}_N)$ spanned by the operators $F_{\boldsymbol{\delta},\boldsymbol{\gamma}}$ such that $C_{\boldsymbol{\delta}\boldsymbol{\gamma}} = S$, and such that for $j \in S^c$, $\delta_j = \zeta_j$ and $\gamma_j = \eta_j$.

(3) For $S = \{1, \dots, N\}$, define $\mathcal{C}_N = \mathrm{span}(\{F_{\boldsymbol{\gamma},\boldsymbol{\gamma}} : \boldsymbol{\gamma} \in \mathcal{V}_N\})$. That is, $\mathcal{C}_N$ is the span of the $F_{\boldsymbol{\delta},\boldsymbol{\gamma}}$ such that $C_{\boldsymbol{\delta}\boldsymbol{\gamma}} = \{1, \dots, \mathbb{N}\}$ in which case there are no exterior configurations to be considered. Note that $\mathcal{C}_N$ is not only a subspace of $\mathcal{B}(\mathcal{H}_N)$, it is a commutative subalgebra of $\mathcal{B}(\mathcal{H}_N)$. It is called the *classical subalgebra of* $\mathcal{B}(\mathcal{H}_N)$.

Lemma 5.2. *The N-particle space H_N is the direct sum of the subspaces $\mathcal{B}_{S;\boldsymbol{\zeta},\boldsymbol{\eta}}$; that is,*

$$\mathcal{B}(\mathcal{H}_N) = \mathcal{C}_N \oplus \Big(\bigoplus_{S \subsetneq \{1,\dots,N\},\ (\boldsymbol{\zeta},\boldsymbol{\eta}) \in E_S} \mathcal{B}_{S;\boldsymbol{\zeta},\boldsymbol{\eta}} \Big). \tag{5.1}$$

Proof. It is evident that, for each $\boldsymbol{\delta}, \boldsymbol{\gamma} \in \mathcal{V}_N$, $F_{\boldsymbol{\delta},\boldsymbol{\gamma}}$ belongs to $\mathcal{B}_{S;\boldsymbol{\zeta},\boldsymbol{\eta}}$ if and only if $S = C_{\boldsymbol{\delta}\boldsymbol{\gamma}}$ and for each $j \notin S$,$\delta_j = \zeta_j$ and $\gamma_j = \eta_j$. Thus, each of the basis vectors $F_{\boldsymbol{\delta},\boldsymbol{\gamma}}$ belongs to exactly one of the spaces $\mathcal{B}_{J;\boldsymbol{\zeta},\boldsymbol{\eta}}$, and this proves (5.1). ∎

For $M \in \mathbb{N}$, let $L^2(\mathcal{G}_M)$ denote the Hilbert space obtained by equipping $\mathcal{G}_M$ with counting measure. For each multi-index $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_M)$, define a function $g_{\boldsymbol{\beta}}$ on $\mathcal{V}_M$ by $g_{\boldsymbol{\beta}}(\boldsymbol{\alpha}) = \delta_{\boldsymbol{\alpha},\boldsymbol{\beta}}$. Then, $\{g_{\boldsymbol{\beta}}\}_{\boldsymbol{\alpha} \in \mathcal{V}_M}$ is an orthonormal basis for $L^2(\mathcal{G}_M)$.

Fix some $S \subsetneq \{1, \dots, N\}$ with cardinality $|S| = M$, and write it in the form $\{j_1, \dots, j_M\}$. Define the map $k_S : S \to \{1, \dots, M\}$ by $k_S(j_k) = k$. In addition, for $M < N$, fix some $(\boldsymbol{\zeta}, \boldsymbol{\eta}) \in E_S$. Then, define a unitary map $U_{S;\boldsymbol{\zeta}\boldsymbol{\eta}}$ from $L^2(\mathcal{G}_M)$ to $\mathcal{B}_{S;\boldsymbol{\zeta},\boldsymbol{\eta}}$ by linearly extending

$$U_{S;\boldsymbol{\zeta}\boldsymbol{\eta}}(g_{\boldsymbol{\beta}}) = F_{\boldsymbol{\gamma},\boldsymbol{\delta}}, \quad \text{where } \begin{cases} \gamma_j = \delta_j = \beta_{k_S(j)}, & j \in S \\ \gamma_j = \zeta_j,\ \delta_j = \eta_j, & j \notin S. \end{cases} \tag{5.2}$$

This map is unitary because it takes an orthonormal basis of $L^2(\mathcal{G}_M)$ to an orthonormal basis of $\mathcal{B}_{S;\boldsymbol{\zeta},\boldsymbol{\eta}}$. For $S = \{1, \dots, N\}$, there is the simpler unitary map $U_{\mathcal{C}_N}$ from $L^2(\mathcal{G}_M)$ onto $\mathcal{C}_N$ defined by $U_{\mathcal{C}_N}(g_{\boldsymbol{\beta}}) = F_{\boldsymbol{\beta}\boldsymbol{\beta}}$.

Theorem 5.3. *Let $S \subsetneq \{1, \dots, N\}$ with $|S| = M$, and let $(\boldsymbol{\zeta}, \boldsymbol{\eta}) \in E_S$. Define $r := N - M$. For all $f \in L^2(\mathcal{G}_M)$, and all $\boldsymbol{\alpha}, \in \mathcal{V}_M$,*

$$U^*_{S;\boldsymbol{\zeta}\boldsymbol{\eta}}(-\mathcal{L}_N)U_{S;\boldsymbol{\zeta}\boldsymbol{\eta}} f(\boldsymbol{\alpha}) = \frac{1}{N-1}\Delta_{\mathcal{G}_M} f(\boldsymbol{\alpha}) + \left(2r\frac{N}{N-1} - \frac{r(r+1)}{N-1}\right) f(\boldsymbol{\alpha}).$$

For $S = \{1, \dots, N\}$, we have

$$U^*_{\mathcal{C}_N}(-\mathcal{L}_N)U_{\mathcal{C}_N} = \frac{2}{N-1}\Delta_{\mathcal{G}_N} f(\boldsymbol{\alpha}).$$

Theorem 5.3 reduces the study of the spectrum of $\mathcal{L}_N$ to the study of the spectrum of the graph Laplacians $\Delta_{\mathcal{G}_M}$, $M \leq N$. The rest of this section is devoted to the proof of Theorem 5.3. In the next section, we turn to the analysis of the spectrum of $\Delta_{\mathcal{G}_M}$, $M \leq N$. We give a new a relatively simple proof of some known relevant facts about the spectrum, and in particular, the determination of the spectral gap.

Proof of Theorem 5.3. Fix $\boldsymbol{\beta} \in \mathcal{G}_M$, and let $F_{\boldsymbol{\gamma},\boldsymbol{\delta}} = U_{S;\boldsymbol{\zeta}\boldsymbol{\eta}}(g_{\boldsymbol{\beta}})$ so that $\boldsymbol{\gamma}$ and $\boldsymbol{\delta}$ are given by (5.2). Then, $C_{\boldsymbol{\gamma},\boldsymbol{\delta}} = M$, and from Theorem 4.1,

$$\begin{aligned} N^{-1}\binom{N}{2}\mathcal{L}_N(F_{\boldsymbol{\gamma}\boldsymbol{\delta}}) &= \frac{1}{2}\sum_{m<n}\delta_{\gamma_m\delta_m}\delta_{\gamma_n\delta_n}[F_{\boldsymbol{\gamma}\boldsymbol{\delta}} + F_{S_{mn}(\boldsymbol{\gamma})S_{mn}(\boldsymbol{\delta})}] - F_{\boldsymbol{\gamma}\boldsymbol{\delta}} \\ &= \frac{1}{2}\sum_{m<n}\delta_{\gamma_m\delta_m}\delta_{\gamma_n\delta_n}[F_{S_{mn}(\boldsymbol{\gamma})S_{mn}(\boldsymbol{\delta})} - F_{\boldsymbol{\gamma}\boldsymbol{\delta}}] \\ &\quad - \left(\binom{N}{2} - \binom{M}{2}\right)F_{\boldsymbol{\gamma}\boldsymbol{\delta}}. \end{aligned}$$

Now, observe that

$$\begin{aligned} &U_{S;\boldsymbol{\zeta}\boldsymbol{\eta}}\left(\frac{1}{2}\sum_{m<n}\delta_{\gamma_m\delta_m}\delta_{\gamma_n\delta_n}[F_{S_{mn}(\boldsymbol{\gamma})S_{mn}(\boldsymbol{\delta})} - F_{\boldsymbol{\gamma}\boldsymbol{\delta}}]\right)U^*_{S;\boldsymbol{\zeta}\boldsymbol{\eta}}(\boldsymbol{\alpha}) \\ &= \sum_{\{\boldsymbol{\alpha}':[\boldsymbol{\alpha},\boldsymbol{\alpha}']\in\mathcal{E}_M\}} g_{\boldsymbol{\beta}}(\boldsymbol{\alpha}') - v(\boldsymbol{\alpha})g_{\boldsymbol{\beta}}(\boldsymbol{\alpha}) = -\Delta_{\mathcal{G}_M}g_{\boldsymbol{\beta}}(\boldsymbol{\alpha}), \end{aligned}$$

and

$$\binom{N}{2} - \binom{M}{2} = \frac{(N^2-N) - (N^2 - (2r+1)N + r(r+1))}{2} = rN - \frac{r(r+1)}{2}.$$

■

6. The spectrum of the Graph Laplacian on the multislice

6.1. The multislice

The graph $\mathcal{G}_N$ is known as the *multislice* in analogy with the sliced Boolean cube $\{0,1\}^N$. The pair-transposition random walk on the vertices of the Boolean cube preserves the sum of the coordinates belonging to a vertex in $\{0,1\}^N$, and hence, the paths of the walk stay in, and eventually cover, the "slices" of $\{0,1\}^N$ corresponding to the $N+1$ possible values of the sum of the coordinates.

When h is non-degenerate, we identify $\mathcal{V}_N = \{1,\dots,d\}^N$ with $\{e_1,\dots,e_d\}^N$. Then, due to energy conservation, our pair transposition walk on $\mathcal{V}_N$ conserves the value of the sum of the coordinates. The possible values of this sum are the eigenvalues of H_N, and we have seen that these are indexed by the occupation vectors $\mathbf{k}(\boldsymbol{\alpha})$,

$\boldsymbol{\alpha} \in \mathcal{G}_N$. Under the strong non-degeneracy condition, there is a one-to-one correspondence between eigenvalues E of H_N, and occupation vectors $\mathbf{k} = (k_1, \dots, k_d)$ such that each k_j is a non-negative integer and $\sum_{j=1}^d k_j = N$. For each such $\mathbf{k}$, define $\mathcal{G}_{N,\mathbf{k}}$ to be the subgraph of $\mathcal{G}_N$ consisting of those vertices $\boldsymbol{\alpha} \in \mathcal{G}_N$ for which $\mathbf{k}(\boldsymbol{\alpha}) = \mathbf{k}$. (This is a slight shift from our previous notation $\mathcal{G}_{N,E}$, but in this purely graph theoretic context, notation referring to $\mathbf{k}$ instead of E is natural.) It is easy to see that these are precisely the connected components of $\mathcal{G}_N$. Thus, $\Delta_{\mathcal{G}_N}$ is the direct sum of the operators $\Delta_{\mathcal{G}_N,\mathbf{k}}$.

Theorem 6.1. *For all $N \geq 2$, all $d \geq 2$, and all $\mathbf{k} = (k_1, \dots, k_d) \in \mathbb{Z}^d_{\geq 0}$ with*

$$\sum_{m=1}^{d} k_m = N \quad \text{and} \quad \max\{k_0, \dots, k_{r-1}\} < N$$

so that $\mathcal{G}_{N,\mathbf{k}}$ is not trivial, the spectral gap $\Gamma_{N,\mathbf{k}}$ of $\Delta_{\mathcal{G}_{N,\mathbf{k}}}$ is given by

$$\Gamma_{N,\mathbf{k}} = N.$$

Granted this, we now prove Theorem 3.7.

Proof of Theorem 3.7. To show that for all $E \in \mathrm{Spec}(H_N)$, such that $\dim(\mathcal{K}_{N,E}) > 1$, $\Gamma_{\mathcal{L}_{N,E}} \geq \frac{N}{N-1}$, it suffices to prove that the least non-zero eigenvalue of $-\mathcal{L}_N$ is $\frac{N}{N-1}$.

By Lemma 5.2 and Theorem 5.3, every eigenvalue of $\mathcal{L}_N$ is of the form

$$\frac{1}{N-1}\lambda + \frac{1}{N-1}(2rN - r(r+1)),$$

where $\lambda \geq 0$ is an eigenvalue of $\Delta_{\mathcal{G}_M} f(\boldsymbol{\alpha})$ and r is an integer in $\{0, \dots, N-1\}$. By concavity,

$$\begin{aligned}\min\{(2rN - r(r+1)) : r \in \{1, \dots, N-1\}\} &= \min\{2(N-1), N(N-1)\} \\ &= 2(N-1).\end{aligned}$$

Therefore, the least eigenvalue in the subspaces corresponding to $r > 0$ is $2\frac{N-1}{N}$.

Next, consider $r = 0$. By Lemma 5.2, this corresponds to invariant subspace $\mathcal{C}_N$; that is the classical sector, since $\mathcal{C}_N$ is a commutative subalgebra of $\mathcal{B}(\mathcal{H}_N)$. For the classical sector, Theorem 5.3 says that $-\mathcal{L}_N$ is unitarily equivalent to $\frac{1}{N-1}\Delta_{\mathcal{G}_N}$. It then follows immediately from Theorem 6.1 that, on this sector, the smallest non-zero eigenvalue of $-\mathcal{L}_N$ is $\frac{N}{N-1} < 2\frac{N-1}{N}$. Therefore, the gap is $\frac{N}{N-1}$, and all gap eigenvectors lie in the classical sector. ∎

Remark 6.2. The proof of Theorem 3.7 not only yields the exact spectral gap for the QKME; it shows that all truly quantum modes decay at least twice as fast as the slowest classical mode.

Turning to the proof of Theorem 6.1, it is easy to write down a set of eigenfunctions of $\Delta_{\mathcal{G}_{N,\mathbf{k}}}$ that have eigenvalue N. This will be very useful in the proof that N is in fact the spectral gap.

Definition 6.3. Let $\mathcal{K}_{N,\mathbf{k}}$ denote the set of real-valued functions g on $\{e_1,\dots,e_d\}$ such that

$$\sum_{m=1}^{d} k_m g(e_m) = 0.$$

Lemma 6.4. *Let g be any non-zero function in $\mathcal{K}_{N,\mathbf{k}}$ as specified in Definition 6.3. Fix $1 \le \ell \le N$ and define a function f on $\mathcal{V}_{N,\mathbf{k}}$ by $f(x) = g(x_\ell)$. Then,*

$$\Delta_{\mathcal{G}_{N,\mathbf{k}}} f(x) = N f(x). \tag{6.1}$$

Proof. Note that $f(x) - f(\pi_{i,j}x) = 0$ unless $i = \ell$ or $j = \ell$; hence, we need only consider such pair permutations when computing $L_{\mathcal{G}_{N,\mathbf{k}}} f(x)$. For any $0 \le m \le r-1$, consider $x \in \mathcal{V}_{N,\mathbf{k}}$ such that $x_\ell = e_m$. For each $n \ne m$, there are k_n pair permutations such that when applied to x yield the value e_n in the ℓth place. Therefore,

$$\begin{aligned}\Delta_{\mathcal{G}_{N,\mathbf{k}}} f(x) &= \sum_{n\ne m} k_n (g(e_m) - g(e_n)) \\ &= (N - k_m) g(e_m) - \sum_{n\ne m} k_n g(e_n) \\ &= (N - k_m) g(e_m) + k_m g(e_x) = N g(e_m) = N f(x),\end{aligned}$$

where in the last line we have used

$$\sum_{n=0}^{r-1} k_n g(e_n) = 0.$$

Since m is arbitrary, (6.1) is proved. ∎

Remark 6.5. Fix any function g on $\{e_1,\dots,e_d\}$ such that $\sum_{n=1}^{d} k_n g(e_n) = 0$. Then, the N functions $\{g(x_1),\dots,g(x_N)\}$ are not linearly independent since, for any $x \in \mathcal{V}_{N,\mathbf{k}}$,

$$\sum_{\ell=1}^{N} g(x_\ell) = \sum_{n=1}^{d} k_n g(e_n) = 0. \tag{6.2}$$

Now, consider any $\{g_1,\dots,g_N\} \subset \mathcal{K}_{M,\mathbf{k}}$, not all zero, and define the function

$$f(x) = \sum_{\ell=1}^{N} g_\ell(x_\ell).$$

By Lemma 6.4, $L_{\mathcal{G}_{N,\mathbf{k}}} f = Nf$. However, we can express f in a simpler way: since by (6.2), $\sum_{\ell=1}^{N} g_N(x_\ell) = 0$,

$$f(x) = f(x) - \left(\sum_{\ell=1}^{N} g_N(x_\ell) \right) = \sum_{\ell=1}^{N-1} h_\ell(x_\ell),$$

where, for $1 \leq \ell \leq N-1$, $h_\ell = g_\ell - g_N$.

6.2. Spectral properties of the graph Laplacian on the multislice

For each N, there is a natural partial order on the set of vectors $\mathbf{k} = (k_1, \ldots, k_d)$ induced by the "coarsening operation" of "merging" energy levels [24]. For any $d' > d \geq 2$, let $\phi : \{0, \ldots, d'\} \to \{0, \ldots, d\}$ be any surjection. For $\mathbf{k} = (k_0, \ldots, k_{d'})$ with $\sum_{n=0}^{d'} k_n = N$, define

$$\phi(\mathbf{k})_m := \sum_{n:\phi(n)=m} k_n \quad \text{and} \quad \phi(\mathbf{k}) = (\phi(\mathbf{k})_1, \ldots, \phi(\mathbf{k})_d).$$

Then, ϕ induces a map, also denoted by ϕ, from $\{e_1, \ldots, e_{d'}\}$ into itself by

$$\phi(e_n) = e_{\phi(n)}, \quad 1 \leq n \leq d'. \tag{6.3}$$

We say that one multislice $\mathcal{V}_{N,\mathbf{k}}$ is *coarser* than another $\mathcal{V}_{N,\mathbf{k}'}$ if, for some $2 \leq d < d' \leq N$, there is a surjection $\phi : \{1, \ldots, d'\} \to \{1, \ldots, d\}$ such that $\phi(\mathbf{k}') = \mathbf{k}$.

In this case, ϕ induces a map from $\mathcal{V}_{N,\mathbf{k}}$ onto $\mathcal{V}_{N,\mathbf{k}'}$ given by

$$(\phi(x))_\ell := \phi(x_\ell) \tag{6.4}$$

with $\phi(x_\ell)$ defined by (6.3).

The relevance of such coarsenings to spectral problems was pointed out and exploited in [12,13]. In our setting, suppose that for some ϕ as above we have $\mathbf{k} = \phi(\mathbf{k}')$. It is easy to see that, for any real-valued function f on $\mathcal{V}_{N,\mathbf{k}}$,

$$(\Delta_{\mathcal{V}_{N,\mathbf{k}}} f) \circ \phi = \Delta_{\mathcal{V}_{N,\mathbf{k}'}} (f \circ \phi).$$

Let f be an eigenfunction of $\Delta_{\mathcal{G}_{N,\mathbf{k}}}$ with eigenvalue λ. Then,

$$\lambda f \circ \phi = (\Delta_{\mathcal{V}_{N,\mathbf{k}}} f) \circ \phi = \Delta_{\mathcal{V}_{N,\mathbf{k}'}} (f \circ \phi).$$

Since the map ϕ defined in (6.4) is surjective, $f \circ \phi$ is not identically zero, and hence, λ is also an eigenvalue of $\Delta_{\mathcal{V}_{N,\mathbf{k}}}$. Therefore, when the multislice $\mathcal{V}_{N,\mathbf{k}}$ is coarser than the multislice $\mathcal{V}_{N,\mathbf{k}'}$, the spectrum of $\Delta_{\mathcal{G}_{N,\mathbf{k}}}$ is contained in the spectrum of $\Delta_{\mathcal{G}_{N,\mathbf{k}'}}$. In particular,

$$\Gamma_{N,\mathbf{k}'} \geq \Gamma_{N,\mathbf{k}}. \tag{6.5}$$

Whenever $\mathcal{G}_{N,\mathbf{k}}$ is not trivial, i.e., has at least one edge, it is known that $\Gamma_{N,\mathbf{k}} = N$, independent of $\mathbf{k}$. This result can be found in [24, Lemma 1], in which the proof refers to the deep proof by Caputo, Liggett, and Richthammer [5] of a famous conjecture of Aldous [2]. This fact about the gap also follows from (6.5) and some computations that follow. Because of (6.5), it suffices to know $\Gamma_{N,\mathbf{k}}$ for a few special choices of $\mathbf{k}$.

Among the graphs considered here, some are absolutely trivial. For example, if $k_m = N$ for some $0 \le m \le r-1$, then $\mathcal{V}_{N,\mathbf{k}}$ is a singleton, and the edge set $\mathcal{E}_{N,\mathbf{k}}$ is empty. In this case, the graph Laplacian is 0, and there is only this one eigenvalue, and hence no gap.

Somewhat less trivial is the case in which $k_{m_0} = N-1$ for some m_0. Then, $k_m = 1$ for one value of $m \neq m_0$, and $k_n = 0$ for all $n \neq m, m_0$. In this case, every vertex is related to every other by a pair transposition, and hence, the graph is a complete graph with N vertices, and therefore, the spectral gap is N.

For $r = 2$, we might as well take $\{e_0, e_1\} = \{0, 1\}$, and then,

$$\{e_0, \dots, e_{r-1}\} = \{0, 1\}^N,$$

the Boolean N-cube. Take $\mathcal{G} = \{0, 1\}^N$ with adjacency defined as above. The connected components $\mathcal{G}_{N(k_0,k_1)}$ are known as *Johnson Graphs*, and the full spectrum of the Laplacian $L_{\mathcal{G}_{N,(k_0,k_1)}}$ is known [3, 15]. In particular, it is known that the spectral gap is always N independent of $\mathbf{k} = (k_0, k_1)$, assuming that both k_0 and k_1 are non-zero.

Finally, consider the case in which $r = N$ and $\mathbf{k} = (1, \dots, 1)$, i.e., $k_m = 1$ for all m. Then, evidently, $\mathcal{V}_{N,(1,\dots,1)}$ has $N!$ vertices and may be identified with S_N, the symmetric group on N letters. The spectrum of the corresponding graph Laplacian $L_{\mathcal{V}_{N,(1,\dots,1)}}$ has been studied using methods from group representation theory by Diaconis and Shahshahani [14]. Their results provide complete information on all of the eigenvalues, and this is essential for their applications. One of their results is that, for all N, the spectral gap is N. For this alone, one does not need so much machinery, and a simple proof is given in [8, Theorem 5.1].

Now, consider any $\mathbf{k}$ such that $\mathcal{G}_{N,\mathbf{k}}$ is non-trivial. Evidently, $\mathbf{k}$ is coarser than

$$\mathbf{k}_1 := (1, \dots, 1),$$

and going in the opposite direction, reducing to just two energies, there is a $\mathbf{k}_0 = (k_0, k_1)$ such that

$$\Gamma_{N,\mathbf{k}_0} \le \Gamma_{N,\mathbf{k}} \le \Gamma_{N,\mathbf{k}_1}.$$

Since $\mathcal{G}_{N,\mathbf{k}_0}$ is a Johnson graph, $\Gamma_{N,\mathbf{k}_0} = N$ [3]. Then, since $\Gamma_{N,\mathbf{k}_1} = N$, $\Gamma_{N,\mathbf{k}} = N$. This result is explicitly noted in [24, Lemma 1], with an argument based on the proof of Aldous' conjecture [2] by Caputo, Liggett, and Richthammer [5].

We now give a simple proof of Theorem 6.1 and somewhat more use ideas developed in [8], applied there to the case of the sliced Boolean cube.

6.3. The induction for the lower bound on the gap

Define $\mu_{N,\mathbf{k}}$ to be the uniform probability measure on $\mathcal{V}_{N,\mathbf{k}}$. The Dirichlet form for $\Delta_{\mathcal{G}_{N,\mathbf{k}}}$ on $L^2(\mu_{N,\mathbf{k}})$ is

$$\frac{1}{2}\sum_{x\in\mathcal{V}_{N,\mathbf{k}}}\sum_{i<j}(f(x)-f(\pi_{i,j}x))^2\mu_{N,\mathbf{k}}. \tag{6.6}$$

It greatly simplifies the induction we will carry out if we normalize so that the sum over pairs becomes an average. Therefore, we will work with the Dirichlet form of $\binom{N}{2}^{-1}\Delta_{\mathcal{G}_{N,\mathbf{k}}}$:

$$\frac{1}{2}\binom{N}{2}^{-1}\sum_{x\in\mathcal{V}_{N,\mathbf{k}}}\sum_{i<j}(f(x)-f(\pi_{i,j}x))^2\mu_{N,\mathbf{k}}. \tag{6.7}$$

The key to our induction is the identity

$$\begin{aligned}&\binom{N}{2}^{-1}\sum_{i<j}(f(\pi_{i,j}x)-f(x))^2\\ &\quad=\frac{1}{N}\sum_{\ell=1}^{N}\left(\binom{N-1}{2}^{-1}\sum_{i<j,i,j\neq\ell}(f(\pi_{i,j}x)-f(x))^2\right).\end{aligned} \tag{6.8}$$

On the right, we have an average of N terms, each of which leaves one coordinate, x_ℓ, unchanged since transpositions $\pi_{i,j}$ in which either $i=\ell$ or $j=\ell$ are not included. If one thinks in terms of processes defined by the Dirichlet forms, this identity will relate the dynamics for N particles to the dynamics for $N-1$ particles.

First, we make one more adjustment to the N particle dynamics. The Dirichlet form (6.7) is associated to a continuous-time Markov jump process on $\mathcal{V}_{N,\mathbf{k}}$ of the following description: a Poisson clock is running with expected times between "rings" equal to 2. When a "ring" occurs, a pair (i,j), $i<j$, is chosen uniformly at random, and the state jumps from vertex x to vertex $\pi_{i,j}x$. For any given $1\le\ell\le N$, the number of pairs $i<j$ containing ℓ is $N-1$, and hence, the fraction of the jumps that change the state of the ℓth particle is $2/N$. In order to have that all particles update with an expected time of order 1, independent of N, we therefore multiply the Dirichlet form in (6.7) by N to obtain a family of processes, indexed by N, in which the expected waiting times for updates of each particle are of order 1, independent of N. This is physically motivated, but as we will see, it is also convenient for the induction.

Definition 6.6. Define the Dirichlet form

$$\mathcal{D}_{N,k}(f,f) = \frac{N}{2}\binom{N}{2}^{-1} \sum_{x\in\mathcal{V}_{N,\mathbf{k}}} \sum_{i<j} (f(\pi_{i,j}x) - f(x))^2 \mu_{N,\mathbf{k}}(x)$$
$$= \frac{1}{N-1} \sum_{x\in\mathcal{V}_{N,\mathbf{k}}} \sum_{i<j} (f(\pi_{i,j}x) - f(x))^2 \mu_{N,\mathbf{k}}(x), \tag{6.9}$$

where the pair permutations $\pi_{i,j}$ acts on x by swapping the i and jth entries. Also, define $\widehat{\Gamma}_{N,\mathbf{K}}$ to be the spectral gap associated to this Dirichlet from; that is,

$$\widehat{\Gamma}_{N,\mathbf{k}} = \inf\big\{\mathcal{D}_{N,k}(f,f) : \|f\|_{L^2(\mu_{N,\mathbf{k}})} = 1,\ \langle f,1\rangle_{L^2(\mu_{N,\mathbf{k}})} = 0\big\}.$$

Remark 6.7. Comparing with (6.6) which gives the Dirichlet form of the graph Laplacian $\Delta_{N,\mathbf{k}}$, we see that its gaps $\Gamma_{N,\mathbf{k}}$ and $\widehat{\Gamma}_{N,\mathbf{k}}$, are related by

$$\widehat{\Gamma}_{N,\mathbf{k}} = \frac{2}{N-1}\Gamma_{N,\mathbf{k}}. \tag{6.10}$$

To make use of (6.8), we first consider a graph $\mathcal{G}_{N,\mathbf{k}}$, where $\mathbf{k} = (k_1,\dots,k_d)$ is such that

$$k_m \geq 1 \quad \text{for each } 1 \leq m \leq d. \tag{6.11}$$

Then, $\mathcal{G}_{N,\mathbf{k}}$ is a graph for N particles that truly have d different energy levels. If it were the case that $k_m = 0$ for some m, the energy e_m would play no role, and the graph would be identical to another graph with a reduced set of $r' < r$ energy levels and a net $\mathbf{k}'$ such that, for all $0 \leq m \leq r'-1$, $k'_m \geq 1$. Evidently, $\mathcal{G}_{N,\mathbf{k}}$ and $\mathcal{G}_{N,\mathbf{k}'}$ are isomorphic and in particular have the same spectral gap.

Now, considering $\mathcal{G}_{N,\mathbf{k}}$ such that (6.11) is satisfied, we specify a bijection of $\mathcal{V}_{N,\mathbf{k}}$ with a union of vertex sets of graphs for $N-1$ particles: for $0 \leq m \leq r-1$, define $\mathbf{k}^{(m)}$ to be obtained from $\mathbf{k}$ by replacing k_m with $k_m - 1$. For each $1 \leq \ell \leq N$, we define a map

$$T_\ell : \left(\bigcup_{m=0}^{r-1} \mathcal{V}_{N-1,\mathbf{k}^{(m)}}\right) \to \mathcal{V}_{N,\mathbf{k}}$$

by

$$T_\ell(x) = (x_1,\dots,x_{\ell-1},e_m,x_\ell,\dots,x_{N-1}) \quad \text{for } x \in \mathcal{V}_{N-1,\mathbf{k}^{(m)}}$$

with the obvious modifications for $\ell = 1$ or $\ell = N-1$. In other words, for $x \in \mathcal{V}_{N-1,\mathbf{k}^{(m)}}$, one simply inserts e_m in the ℓth place, keeping the order of the remaining entries unchanged, and thus obtains an element of $\mathcal{V}_{N,\mathbf{k}}$. It is evident that this does indeed yield a bijection. The set $\{x \in \mathcal{V}_{N,\mathbf{k}} : x_\ell = e_m\}$ is precisely the image of $\mathcal{V}_{N-1,\mathbf{k}^{(m)}}$ under T_ℓ. We will prove the following theorem.

Theorem 6.8. *Let $\{e_1, \dots, e_d\}$ be given along with $\mathbf{k} = (k_0, \dots, k_{r-1})$, where each k_m is a strictly positive integer and $\sum_{m=1} k_m = N$. Then, the spectral gap $\Delta_{N,\mathbf{k}}$ for the corresponding Dirichlet form specified in (6.9) satisfies*

$$\widehat{\Gamma}_{N,\mathbf{k}} \geq \frac{N(N-2)}{(N-1)^2} \min\{\widehat{\Gamma}_{N-1,\mathbf{k}^{(m)}} : 0 \leq m \leq r-1\}.$$

We will prove this to be a consequence of several lemmas and begin by explaining how we make use of (6.8)

For each $1 \leq \ell \leq N$, and each $m \in \{0, \dots, r-1\}$, define

$$\begin{aligned}
&\mathcal{D}^{\ell,m}_{N,\mathbf{k}}(f,f) \\
&= \frac{N-1}{2}\binom{N-1}{2}^{-1} \sum_{x \in \mathcal{V}_{N,\mathbf{k}}, x_\ell = e_m} \Big(\sum_{i<j, i, j \neq \ell} (f(\pi_{i,j}x) - f(x))^2 \Big) \mu_{N-1,\mathbf{k}^{(m)}} \\
&= \frac{1}{N-2} \sum_{x \in \mathcal{V}_{N,\mathbf{k}}, x_\ell = e_m} \Big(\sum_{i<j, i, j \neq \ell} (f(\pi_{i,j}x) - f(x))^2 \Big) \mu_{N-1,\mathbf{k}^{(m)}}.
\end{aligned}$$

Next, for each $1 \leq \ell \leq N$, define the operator P_ℓ on $L^2(\mathcal{V}_{N,\mathbf{k}})$ as follows: on the set $\{x : x_\ell = e_m\}$,

$$P_\ell f(x) := \mu_{N,\mathbf{k}^{(m)}} \sum_{y \in \mathcal{V}_{N,\mathbf{k}} : y_\ell = e_m} f(y).$$

The operator P_ℓ is just the orthogonal projection in $L^2(\mu_{N,\mathbf{k}})$ onto the subspace of functions that depend only on x_ℓ. Therefore, for each $m \in \{0, \dots, r-1\}$,

$$\mathcal{D}^{\ell,m}_{N,\mathbf{k}}(f,f) = \mathcal{D}^{\ell,m}_{N,\mathbf{k}}(f - P_\ell f, f - P_\ell f). \tag{6.12}$$

Also, note that

$$\mu_{N,\mathbf{k}} = \sum_{m=0}^{r-1} \frac{k_m}{N} \mu_{N-1,\mathbf{k}^{(m)}}. \tag{6.13}$$

Therefore, using the key identity (6.8), together with (6.12) and (6.13),

$$\mathcal{D}_{N,\mathbf{k}}(f,f) = \frac{1}{N} \sum_{\ell=1}^{N} \frac{N}{N-1} \sum_{m=0}^{r-1} \mathcal{D}^{\ell,m}_{N,\mathbf{k}}(f - P_\ell f, f - P_\ell f) \frac{k_m}{N}. \tag{6.14}$$

Recall that $\widehat{\Gamma}_{N,\mathbf{k}}$ is the spectral gap of the Dirichlet form defined in (6.9). Since for each $m = 0, \dots, r-1$, $f - P_\ell f$ is constant on the image of each $\mathcal{V}_{N-1,\mathbf{k}^{(m)}}$ under T_ℓ,

$$\mathcal{D}^{\ell,m}_{N,\mathbf{k}}(f - P_\ell f, f - P_\ell f) \geq \Delta_{N-1,\mathbf{k}^{(m)}} \|(f - P_\ell f) \circ T_\ell\|^2_{L^2(\mu_{N-1,\mathbf{k}^{(m)}})}.$$

By (6.13), and the fact that each P_ℓ is an orthogonal projection,

$$\sum_{m=1}^{r-1} \|(f - P_\ell f) \circ T_\ell\|^2_{L^2(\mu_{N-1,\mathbf{k}(m)})} \frac{k_m}{N} = \|f - P_\ell f\|_{L^2(\mu_{N,\mathbf{k}})} \\ = \|f\|^2_{L^2(\mu_{N,\mathbf{k}})} - \langle f, P_\ell f\rangle_{L^2(\mu_{N,\mathbf{k}})}.$$

Then, taking f to be a normalized gap eigenfunction for $\Delta_{N,\mathbf{k}}$, we have from (6.14) that

$$\widehat{\Gamma}_{N,\mathbf{k}} \geq \min\{\widehat{\Gamma}_{N-1,\mathbf{k}(m)} : 0 \leq m \leq r-1\} \frac{N}{N-1}(1 - \langle f, Pf\rangle_{L^2(\mu_{N,\mathbf{k}})}), \tag{6.15}$$

where

$$P = \frac{1}{N}\sum_{\ell=1}^{N} P_\ell.$$

Note that P is an average of orthogonal projections, and hence, its spectrum lies in $[0, 1]$. Any function f that is an eigenvalue of P with the eigenvalue 1 must be in the range of each of the projections P_ℓ. However, the range of P_ℓ consists of functions f that depend on x only through x_ℓ. For $N \geq 3$, the only functions f on $\mathcal{V}_{N,\mathbf{k}}$ that have this property for all ℓ are the constant functions since, for every $x, y \in \mathcal{V}_{N,\mathbf{k}}$, there is a sequence of pair transpositions that takes x to y, and since $N \geq 3$, each such transposition leaves one coordinate unchanged, and hence leaves the value of f unchanged. Hence,

$$f(x) = f(y).$$

Therefore, for $N \geq 3$, 1 is an eigenvalue of P of multiplicity one with the eigenspace being the constant functions. Since the gap eigenfunction f is orthogonal to the constants in $L^2(\mu_{N,\mathbf{k}})$, we must have

$$\langle f, Pf\rangle < 1.$$

In fact, this quantity can be no larger than the next largest eigenvalue of P.

Definition 6.9. Let $N \geq 3$, and let $\lambda_{N,\mathbf{k}}$ denote the second largest eigenvalue of P

$$\lambda_{N,\mathbf{k}} = \sup\{\langle h, Ph\rangle_{L^2(\mu_{N,\mathbf{k}})} : \|h\|_{L^2(\mu_{N,\mathbf{k}})} = 1,\ \langle h, 1\rangle_{L^2(\mu_{N,\mathbf{k}})} = 0\}.$$

Therefore, (6.15) becomes

$$\widehat{\Gamma}_{N,\mathbf{k}} \geq \min\{\widehat{\Gamma}_{N-1,\mathbf{k}(m)} : 0 \leq m \leq r-1\} \frac{N}{N-1}(1 - \lambda_{N,\mathbf{k}}). \tag{6.16}$$

The next lemma renders (6.16) completely explicit and yields the proof of Theorem 6.8.

Lemma 6.10. *Let $N \geq 3$. The spectrum of P is the set $\{0, (N-1)^{-1}, 1\}$. In particular,*

$$\lambda_{N,\mathbf{k}} = \frac{1}{N-1}. \tag{6.17}$$

Moreover, the eigenspace corresponding to 1 consists of the constant functions, and the eigenspace corresponding to $(N-1)^{-1}$ has dimension $(r-1)(N-1)$ and a basis for it is the set of functions of the form

$$f_{m,\ell}(x) = g_m(x_\ell), \quad 1 \leq m \leq r-1, \quad \text{and} \quad 1 \leq \ell \leq N-1,$$

where $\{g_1, \dots, g_{r-1}\}$ is a basis for $\mathcal{K}_{N,\mathbf{k}}$.

The proof of Lemma 6.10 that we give is patterned on the proof of [6, Lemma 2.16]. It involves a simpler operator K that, like P, is constructed out of the projections P_ℓ. K is an operator on functions of a single variable in $\{e_1, \dots, e_d\}$: let $\nu_{N,\mathbf{k}}$ denote the probability measure on $\{e_1, \dots, e_d\}$ that is the image of the uniform probability measure on $\mathcal{V}_N$ under the map $\pi_N : (x_1, \dots, x_N) \mapsto x_N$. It is easy to see that

$$\nu_{N,\mathbf{k}}(\{e_m\}) = \frac{k_m}{N}.$$

Define the operator K on $L^2(\nu_{N,\mathbf{k}})$ by $Kh = P_1 h \circ \pi_N$. Note that, for any function h on $\{e_1, \dots, e_d\}$, $h \circ \pi_N$ is a function on $\mathcal{V}_N$, depending only on the Nth coordinate, and then, $P_1 h \circ \pi_N$, which is a function of the first coordinate only, may be identified with a function on $\{e_1, \dots, e_d\}$, and this function is, by definition, Kh. There is nothing special about 1 and N, and pairs of distinct indices yield the same operator by symmetry.

By the definition of $\nu_{N,\mathbf{k}}$ in terms of $\mu_{N,\mathbf{k}}$, we have the following formula for K which shows that it is self-adjoint on $L^2(\nu_{N,\mathbf{k}})$:

$$\langle g, Kh \rangle_{L^2(\nu_{N,\mathbf{k}})} := \sum_{x \in \mathcal{V}_{N,\mathbf{k}}} g(x_1) h(x_N) \mu_{N,\mathbf{k}}(x). \tag{6.18}$$

Lemma 6.11. *The spectrum of the K on $L^2(\nu_{N,\mathbf{k}})$ is $\{1, -1/(N-1)\}$. The eigenspace corresponding to the eigenvalue 1 consists of the constant functions on $\{e_0, \dots, e_{r-1}\}$, and the eigenspace corresponding to the eigenvalue $-1/(N-1)$ is the space consisting of functions g on $\{e_0, \dots, e_{r-1}\}$ such that*

$$\sum_{m=1}^{r-1} k_m g(e_m) = 0.$$

Proof. Since, for $m \neq n$, there are $\frac{(N-2)!}{k_0! \cdots k_{r-1}!} k_m k_n$ vertices with $x_1 = e_m$ and $x_N = e_n$, and there are $\frac{(N-2)!}{k_0! \cdots k_{r-1}!} k_m (k_m - 1)$ vertices with $x_1 = x_N = e_m$, working from the

right-hand side of (6.18), we find

$$\sum_{x\in\mathcal{V}_{N,\mathbf{k}}} g(x_1)h(x_N)\mu_{N,\mathbf{k}}(x) = \frac{1}{N(N-1)}\sum_{m=0}^{r-1} g(e_m)h(e_m)k_m(k_m-1) + \frac{1}{N(N-1)}\sum_{m\neq n} g(e_m)h(e_n)k_mk_n.$$

From here, it follows easily that $Kh(e_m) = \sum_{n=0}^{r-1} K_{m,n}h(e_n)$, where

$$(N-1)K_{m,n} = \begin{cases} k_n - 1, & n = m, \\ k_n, & n \neq m. \end{cases}$$

Therefore, $(N-1)K = -1 + L$, where L is the rank one matrix, each of whose rows is $(k_0, \dots, k_{r-1})$. Evidently, the non-zero constant vectors are eigenvectors of K with eigenvalue 1, and every non-zero vector orthogonal to the constants in $L^2(\nu_{N,\mathbf{k}})$ is an eigenvector with eigenvalue $-1/(N-1)$. ∎

Note that the space $\mathcal{K}_{N,\mathbf{k}}$ that figures in Theorem 6.1 is precisely the eigenspace of K corresponding to the eigenvalue $-1/(N-1)$.

We have seen in Remark 6.5 that, for $\{g_1, \dots, g_N\} \subset \mathcal{K}_{N,\mathbf{k}}$, $\{g_1(x_1), \dots, g_N(x_N)\}$ need not be linearly independent even if each g_ℓ is non-zero. The following lemma shows that the only way linear independence can fail is the way indicated in Remark 6.5

Lemma 6.12. *Let $\{g_1, \dots, g_N\} \subset \mathcal{K}_{N,\mathbf{k}}$ Then, $\sum_{\ell=1}^N g_\ell(x_\ell) = 0$ for all $x \in \mathcal{V}_{N,\mathbf{k}}$ if and only if all of the functions $g_1, \dots, g_N$ are the same.*

Proof. By what is explained in Remark 6.5, it suffices to show that if $\sum_{\ell=1}^N g_\ell(x_\ell) = 0$ for all $x \in \mathcal{V}_{N,\mathbf{k}}$, then all of the functions $g_1, \dots, g_N$ are the same. Hence, we assume $\sum_{\ell=1}^N g_\ell(x_\ell) = 0$ and compute

$$\begin{aligned} 0 = \Big\| \sum_{\ell=1}^N g_\ell(x_\ell) \Big\|^2_{L^2(\mu_{N,\mathbf{k}})} &= \sum_{i=1}^N \Big(\|g_i\|^2_{L^2(\nu_{N,\mathbf{k}})} + \sum_{\ell\neq i} \langle g_i, Kg_\ell\rangle_{L^2(\nu_{N,\mathbf{k}})} \Big) \\ &= \sum_{i=1}^N \Big(\|g_i\|^2_{L^2(\nu_{N,\mathbf{k}})} - \frac{1}{N-1}\sum_{\ell\neq i} \langle g_i, g_\ell\rangle_{L^2(\nu_{N,\mathbf{k}})} \Big) \\ &\geq \sum_{i=1}^N \Big(\|g_i\|^2_{L^2(\nu_{N,\mathbf{k}})} - \frac{1}{N-1}\sum_{\ell\neq i} \|g_i\|_{L^2(\nu_{N,\mathbf{k}})}\|g_\ell\|_{L^2(\nu_{N,\mathbf{k}})} \Big) \\ &\geq \sum_{i=1}^N \Big(\|g_i\|^2_{L^2(\nu_{N,\mathbf{k}})} - \frac{1}{N-1}\sum_{\ell\neq i} \frac{1}{2}(\|g_i\|^2_{L^2(\nu_{N,\mathbf{k}})} + \|g_\ell\|^2_{L^2(\nu_{N,\mathbf{k}})}) \Big) = 0. \end{aligned}$$

Hence, both inequalities must be equalities. The first inequality is the Schwarz inequality and a worst-case assumption on the signs, and equality here entails that the functions $g_1, \dots, g_N$ are all positive multiples of one another. The second inequality is the arithmetic-geometric mean inequality, and equality here entails that

$$\|g_i\|_{L^2(\nu_{N,\mathbf{k}})} = \|g_\ell\|_{L^2(\nu_{N,\mathbf{k}})}$$

for all i and ℓ. ∎

Proof of Lemma 6.10. Suppose that f is an eigenfunction of P with eigenvalue $\lambda > 0$. Write

$$P_\ell f(x) =: h_\ell(x_\ell) = h_\ell \circ \pi_\ell(x),$$

where $\pi_\ell(x) = x_\ell$. Define $\vec{h} := (h_1, \dots, h_N)$ viewed as an element of $\mathbb{C}^N \otimes L^2(\nu_{N,\mathbf{k}})$. Since f is an eigenfunction of P, $f \neq 0$ and $N\lambda \sum_{\ell=1}^N h_\ell(x_\ell) = f(x)$. Therefore, $\vec{h} \neq 0$, and the map $f \mapsto \vec{h}$ is injective from the eigenspace of P corresponding to eigenvalue $\lambda > 0$ into $\mathbb{C}^N \otimes L^2(\nu_{N,\mathbf{k}})$. Since this is true for every eigenvalue $\lambda > 0$ of P, the map $f \mapsto \vec{h}$ is injective from $\ker(P)^\perp$ into $\mathbb{C}^N \otimes L^2(\nu_{N,\mathbf{k}})$.

Applying P_i to both sides of $\lambda f = Pf$, and using the formula $Kh_\ell = P_i h_\ell \circ \pi_\ell$,

$$(N\lambda - 1)h_i = \sum_{\ell \neq i} Kh_\ell. \tag{6.19}$$

Define M to be the $N \times N$ matrix with $M_{i,\ell} = \begin{cases} 0 & i = \ell \\ 1 & i \neq \ell \end{cases}$. Then, since (6.19) is valid for each i, we have

$$(N\lambda - 1)\vec{h} = M \otimes K\vec{h}.$$

Since $\vec{h} \neq 0$, $(N\lambda - 1)$ is an eigenvalue of $M \otimes K$. Evidently, the spectrum of M is $\{-1, N-1\}$, and by Lemma 6.11, the spectrum of K is $\{1, -1/(N-1)\}$. Then, the spectrum of $M \otimes K$ is $\{-1, 1/(N-1), N-1\}$. It follows that if $\lambda > 0$, then either $\lambda = 1$ or $\lambda = 1/(N-1)$. Since $(N\lambda - 1) \in \{-1, 1/(N-1), N-1\}$ is equivalent to

$$\lambda \in \{0, 1/(N-1), 1\},$$

this proves that the only eigenvalue λ of P with $0 < \lambda < 1$ is $\lambda = 1/(N-1)$, and hence, (6.17) is proved.

Moreover, we have seen that the map $f \mapsto \vec{h} = (h_1, \dots, h_N)$ is injective from the $1/(N-1)$ eigenspace of P into the $1/(N-1)$ eigenspace of $M \otimes K$, and this eigenspace is the product of the -1 eigenspace of M and the $-1/(N-1)$ eigenspace of K. Evidently, the dimension of this eigenspace is $(N-1)(r-1)$. Hence, the dimension of the $1/(N-1)$ eigenspace of P cannot have a dimension any higher than this.

To see that it is not any lower, consider any non-zero $g \in \mathcal{K}_{N,\mathbf{k}}$, and any $1 \le \ell \le N$, and let $f(x) = g(x_\ell)$. We then compute

$$Pf(x) = \frac{1}{N}\Big(g(x_\ell) + \sum_{i\neq\ell} Kg(x_i)\Big) = \frac{1}{N}\left(g(x_\ell) - \frac{1}{N-1}\sum_{i\neq\ell} g(x_i)\right)$$
$$= \frac{1}{N}\left(\frac{N}{N-1}g(x_\ell) - \frac{1}{N-1}\sum_{i=1}^{N} g(x_i)\right) = \frac{1}{N-1}g(x_\ell) = \frac{1}{N-1}f(x).$$

Hence, all such functions belong to the eigenspace corresponding to the eigenvalue $1/(N-1)$. Choose a basis $\{g_1, \dots, g_{r-1}\}$ of $\mathcal{K}_{N,\mathbf{k}}$. Let f be a non-trivial linear combination of the $(N-1)(r-1)$ functions $f_{m,\ell} = g_m(x_\ell)$, $1 \le m \le r-1$ and $1 \le \ell \le N-1$. The result is a function of the form $\sum_{\ell=0} h_\ell(x_\ell)$ with each $h_\ell \in \mathcal{K}_{N,\mathbf{k}}$, at least one of which is non-zero. Then, by Lemma 6.12, this cannot vanish identically, and hence, the specified set of $(N-1)(r-1)$ functions is linearly independent. Hence, they constitute a basis for the eigenspace corresponding to the eigenvalue $1/(N-1)$ eigenspace corresponding to the eigenvalue $1/(N-1)$ ∎

Proof of Theorem 6.8. This now follows directly from (6.16) and (6.17). ∎

6.4. Proof of Theorem 6.1

To use our inductive relation (6.16), we need to know the values of $\Gamma_{N,\mathbf{k}}$ for small N. For some values of $\mathbf{k}$, this is trivial even for large N: if $\max\{k_m : 0 \le m \le r-1\} = N$, $\mathcal{G}_{N,\mathbf{k}}$ has a single vertex and no edges. We exclude these trivial cases, and going forward suppose that

$$\max\{k_m : 0 \le m \le r-1\} \le N-1. \tag{6.20}$$

If there is equality in (6.20), then every vertex $x = (x_1, \dots, x_N)$ in $\mathcal{V}_{N,\mathbf{k}}$ has all but one of the entries x_j the same, and exactly one that is not. All of these are related to one another by a pair transposition, and hence, in this case, $\mathcal{G}_{N,\mathbf{k}}$ is a complete graph with N vertices, and hence,

$$\Gamma_{N,\mathbf{k}} = N \quad \text{and} \quad \hat{\Gamma}_{N,\mathbf{k}} = \frac{2N}{N-1}$$

for all such k.

Finally, as we have observed before, it suffices to consider graphs $\mathcal{G}_{N,\mathbf{k}}$ for which $k_m \ge 1$ for $0 \le m \le r-1$, since otherwise the graph is the same as one with a smaller set of energies that does satisfy such a condition.

Consider $N = 2$. The only non-trivial choice for $\mathbf{k}$ is with $r = 2$ and $\mathbf{k} = (1,1)$. There are two vertices (e_0, e_1) and (e_1, e_0) and the single edge connects them. This is

a complete graph, and hence, $\Gamma_{2,(1,1)} = 2$ and $\widehat{\Gamma}_{2,(1,1)} = 4$. In summary, for $N = 2$, there is only one non-trivial choice of $\mathbf{k}$, and for this choice, $\widehat{\Gamma}_{2,\mathbf{k}} = 4$.

Next, consider $N = 3$. The non-trivial choices for $\mathbf{k}$ are, with $r = 2$, $\mathbf{k} = (1, 2)$ and $\mathbf{k} = (2, 1)$, both of which are complete graphs, and for $r = 3$, $\mathbf{k} = (1, 1, 1)$. By Theorem 6.8,

$$\widehat{\Gamma}_{3,(1,1,1)} \geq \frac{3}{4} \min\{\widehat{\Gamma}_{2,(0,1,1)}, \widehat{\Gamma}_{2,(1,0,1)}, \widehat{\Gamma}_{2,(1,1,0)}\}.$$

But evidently, $\widehat{\Gamma}_{2,(0,1,1)} = \widehat{\Gamma}_{2,(1,0,1)} = \widehat{\Gamma}_{2,(1,1,0)} = \widehat{\Gamma}_{2,(1,1)} = 4$. Therefore,

$$\widehat{\Gamma}_{3,(1,1,1)} \geq \frac{3}{4}4 = 3.$$

Since $\mathscr{G}_{3,(2,1)}$ and $\mathscr{G}_{3,(1,2)}$ are complete, $\Gamma_{3,(2,1)} = \Gamma_{3,(1/2)} = 3$, and since

$$2/(N-1) = 1$$

for $N = 3$, we also have $\widehat{\Gamma}_{3,(2,1)} = \widehat{\Gamma}_{3,(1,2)} = 3$. In summary, for $N = 3$ and all non-trivial choices of $\mathbf{k}$, $\widehat{\Gamma}_{3,\mathbf{k}} = 3$.

Proof of Theorem 6.1. Let $N \geq 3$ be an integer. We make the inductive hypothesis that, for $M = N - 1$, $\widehat{\Gamma}_{M,\mathbf{k}} = 2M/(M-1)$ for all $\mathbf{k}$ such that $\mathscr{G}_{M,\mathbf{k}}$ is non-trivial. By the remarks made above, this is valid for $M = 2$ and $M = 3$. Now, consider $\mathbf{k}$ such that $\mathscr{G}_{N,\mathbf{k}}$ is non-trivial and such that $k_m \geq 1$ for $0 \leq m \leq r - 1$ which, as explained above, we may assume without loss of generality. Then, by Theorem 6.8, (6.16) and the inductive hypothesis yield

$$\widehat{\Gamma}_{N,\mathbf{k}} \geq \frac{N(N-2)}{(N-1)^2} \frac{2(N-1)}{N-2} = \frac{2N}{N-1}.$$

However, by Lemma 6.4 and (6.10),

$$\widehat{\Gamma}_{N,\mathbf{k}} \leq \frac{2N}{N-1} \quad \text{and hence } \widehat{\Gamma}_{N,\mathbf{k}} = \frac{2N}{N-1}$$

for all N and all $\mathbf{k}$ such that $\mathscr{G}_{N,\mathbf{k}}$ is non-trivial. By (6.10) once more, this proves that $\Gamma_{N,\mathbf{k}} = N$ for all N and all $\mathbf{k}$ such that $\mathscr{G}_{N,\mathbf{k}}$ is non-trivial.

Now, take f to a normalized gap eigenfunction for $\widehat{\Gamma}_{N,\mathbf{k}}$. We have from (6.15) that if f is not a gap eigenfunction of P, there is strict inequality in (6.16), and this in turn would yield

$$\widehat{\Gamma}_{N,\mathbf{k}} > \frac{N(N-2)}{(N-1)^2} \frac{2(N-1)}{N-2} = \frac{2N}{N-1}.$$

This contradiction shows that every gap eigenfunction for $\mathcal{L}_{N,\mathbf{k}}$ is a gap eigenfunction of P. However, Lemma 6.10 provides a complete description of the gap eigenspace of P, and Lemma 6.4 shows that every gap eigenfunction of P is a gap eigenfunction of $\mathcal{L}_{N,\mathbf{k}}$. ∎

7. Relative entropy dissipation

Again, consider our Kac model with strongly non-degenerate spectrum and uniform collision law. Let $E \in \mathrm{Spec}(H_N)$, and let $\tau_{N,E}$ denote the normalized trace on $\mathcal{K}_{N,E}$. That is, for $X \in \mathcal{B}(\mathcal{H}_{N,E})$,

$$\tau_{N,E}(X) := \frac{1}{\dim(\mathcal{H}_{N,E})} \mathrm{Tr}[X].$$

We say that $\varrho \in \mathcal{B}(\mathcal{H}_{N,E})$ is a *normalized density matrix* in case $\varrho \geq 0$ and

$$\tau_{N,E}(\varrho) = 1.$$

Every quantum state on $\mathcal{B}(\mathcal{H}_{N,E})$ has a representation of the form $X \mapsto \tau_{N,E}(X\varrho)$ for some uniquely determined normalized density matrix ϱ.

Recall that $P_{N,E}$ is the orthogonal projection onto $\mathcal{K}_{N,E}$. Then, $P_{N,E}$ is a normalized density matrix in $\mathcal{B}(\mathcal{H}_{N,E})$, and as we have seen, $\mathcal{L}_{N,E}(P_{N,E}) = 0$. That is, $P_{N,E}$ is the equilibrium normalized state in the sector $\mathcal{B}(\mathcal{H}_{N,E})$.

The relative entropy of ϱ with respect to the equilibrium state $P_{N,E}$ is the quantity

$$D(\varrho||P_{N,E}) := \tau_{N,E}(\varrho(\log\varrho - \log P_{N,E})) = \tau_{N,E}(\varrho\log\varrho).$$

The are entropy inequalities that are very useful for studying the approach to equilibrium and that which imply a spectral gap inequality. In our context, these inequalities take the following form: let $C_{N,E}$ be the such that

$$\mathrm{Tr}[\varrho\log\varrho] \leq -C_{N,E}\,\mathrm{Tr}[\log\varrho\mathcal{L}_{N,E}\varrho] \tag{7.1}$$

for all normalized density matrices ϱ in $\mathcal{B}(\mathcal{H}_{N,E})$.

In this case, we have that, for any normalized density matrix ϱ_0,

$$D(e^{t\mathcal{L}_{N,E}}\varrho_0||P_{N,E}) \leq e^{-tC_{N,E}}D(\varrho_0||P_{N,E}).$$

The inequality (7.1) is known as a *modified logarithmic Sobolev inequality*.

The existence of a finite constant $C_{N,E}$ such that (7.1) holds is trivial, but determining the dependence on E and N is not. In the classical sector, or, what is the same thing, for the corresponding walk on slices of the multislice, it is known that $1/2 \leq C_{N,E} \leq 1$ for all non-trivial E and N. See [24, Section 3.4], where this is deduced from a comparison argument and a result of Caputo, Dai Pra, and Posta [4]. It is natural to conjecture that a similar result is valid for the quantum model, and this is the subject of current research.

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