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Complete positivity and self-adjointness

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ABSTRACT

We specify the structure of completely positive operators and quantum Markov semigroup generators that are symmetric with respect to a family of inner products, also providing new information on the order structure and extreme points in some previously studied cases.

1. Introduction

1.1. The setting and notation

Let $\mathcal{M}_N(\mathbb{C})$ denote the set of $N \times N$ matrices over $\mathbb{C}$, $N \geq 2$. Let $\mathfrak{S}_+$ denote the set of non-degenerate density matrices in $\mathcal{M}_N(\mathbb{C})$. That is, each $\sigma \in \mathfrak{S}_+$ is a positive definite $N \times N$ matrix with unit trace. The GNS inner product on $\mathcal{M}_N(\mathbb{C})$ is defined by

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$$\langle B, A\rangle_{GNS} = \mathrm{Tr}[B^* A\sigma] \ . \tag{1.1}$$

Here we are concerned with a family of inner products on $\mathcal{M}_N(\mathbb{C})$ that all reduce to $\langle B, A\rangle_{GNS}$ when either A or B commutes with σ. Let $\mathcal{P}[0,1]$ denote the set of probability measures on the interval $[0,1]$.

1.1 Definition. For each $m \in \mathcal{P}[0,1]$, $\langle\cdot,\cdot\rangle_m$ denotes the inner product on $\mathcal{M}_N(\mathbb{C})$ given by

$$\langle B, A\rangle_m = \mathrm{Tr}[B^* \mathcal{M}_m(A)] \quad \text{where} \quad \mathcal{M}_m(A) = \int_0^1 \sigma^s A \sigma^{1-s} \, \mathrm{d}m(s) \ . \tag{1.2}$$

Notice that for each $s \in [0,1]$,

$$\mathrm{Tr}[B^* \sigma^{1-s} A \sigma^s] = \mathrm{Tr}[(\sigma^{(1-s)/2} B \sigma^{s/2})^* \sigma^{(1-s)/2} A \sigma^{s/2}] \ ,$$

and this quantity is strictly positive when $B = A \neq 0$, and hence $\langle\cdot,\cdot\rangle_m$ is a non-degenerate inner product for every m.

We call the measure m and its associated inner product $\langle\cdot,\cdot\rangle_m$ *even* when m is symmetric with respect to reflection about $s = 1/2$:

$$m(U) = m(1-U) \quad \text{for all measurable } U \subseteq [0,1] \ . \tag{1.3}$$

Note that the GNS inner product corresponds to $m = \delta_0$, the point mass at $s = 0$. Other cases are known by name. Taking $m = \delta_{1/2}$ yields the *Kubo-Martin-Schwinger* (KMS) inner product

$$\langle B, A\rangle_{KMS} = \mathrm{Tr}[B^* \sigma^{1/2} A \sigma^{1/2}] \ . \tag{1.4}$$

Taking m to be uniform on $[0,1]$ yields the *Bogoliubov-Kubo-Mori* (BKM) inner product,

$$\langle B, A\rangle_{BKM} = \int_0^1 \mathrm{Tr}[B^* \sigma^s A \sigma^{1-s}] \mathrm{d}s \ . \tag{1.5}$$

Unlike the GNS inner product, these two are even.

Finally, if $\sigma = N^{-1}\mathbf{1}$, the normalized identity, all choices of m reduce to the normalized Hilbert-Schmidt inner product. Throughout this paper, $\mathfrak{H}$ always denotes the Hilbert space $\mathcal{M}_N(\mathbb{C})$ equipped with this inner product,

$$\langle B, A\rangle_{\mathfrak{H}} = \frac{1}{N}\mathrm{Tr}[B^* A] \ . \tag{1.6}$$

Let $\mathcal{L}(\mathcal{M}_N(\mathbb{C}))$ denote the linear operators on $\mathcal{M}_N(\mathbb{C})$, or, what is the same thing in this finite dimensional setting, on $\mathfrak{H}$. Throughout this paper, a dagger is always used to denote the adjoint with respect to the inner product on $\mathfrak{H}$. That is, for $\Phi \in \mathcal{L}(\mathcal{M}_N(\mathbb{C}))$, $\Phi^\dagger$ is defined by

$$\langle \Phi^\dagger(B), A\rangle_{\mathfrak{H}} = \langle B, \Phi(A)\rangle_{\mathfrak{H}} \tag{1.7}$$

for all A, B. We can also make $\mathcal{L}(\mathcal{M}_N(\mathbb{C}))$ into a Hilbert space by equipping it with the normalized Hilbert-Schmidt inner product. Throughout this paper, this Hilbert space is denoted by $\widehat{\mathfrak{H}}$. The following formula for the inner product in $\widehat{\mathfrak{H}}$ is often useful. Let $\{F_{i,j}\}_{1\leq i,j\leq N}$ be any orthonormal basis for $\mathfrak{H}$. Then for Φ and $\Psi \in \widehat{\mathfrak{H}}$,

$$\langle \Psi, \Phi\rangle_{\widehat{\mathfrak{H}}} = \frac{1}{N^2}\sum_{i,j=1}^{N} \langle \Psi(F_{i,j}), \Phi(F_{i,j})\rangle_{\mathfrak{H}} \ . \tag{1.8}$$

To each $\sigma \in \mathfrak{S}_+$, there corresponds the *modular operator* Δ on $\mathfrak{H}$ defined by

$$\Delta A = \sigma A \sigma^{-1} \ . \tag{1.9}$$

Let $\{u_1, \dots, u_N\}$ be an orthonormal basis of $\mathbb{C}^N$ consisting of eigenvectors of σ, so that for $1 \leq j \leq N$, $\sigma u_j = \lambda_j u_j$. For $1 \leq i, j \leq N$, define $E_{i,j} = \sqrt{N}|u_i\rangle\langle u_j|$, so that $\{E_{i,j}\}_{1\leq i,j\leq N}$ is an orthonormal basis of $\mathfrak{H}$. Then a simple computation shows that for each i, j,

$$\Delta E_{i,j} = \lambda_i \lambda_j^{-1} E_{i,j} \ . \tag{1.10}$$

Thus Δ is diagonalized, with positive diagonal entries, by an orthonormal basis in $\mathfrak{H}$. It follows that Δ is a positive operator on $\mathfrak{H}$. Using the Spectral Theorem, we may then define Δ^s for all s. This provides another way to write the operator $\mathcal{M}_m$ defined in (1.2):

$$\mathcal{M}_m = \left(\int_0^1 \Delta^s \mathrm{d}m\right) R_\sigma \tag{1.11}$$

where R_σ denotes right multiplication by σ, also a positive operator on $\mathfrak{H}$ that commutes with Δ, and hence with $\int_0^1 \Delta^s \mathrm{d}m$.

Finally, the terms "Hermitian" and "self-adjoint" are often used interchangeably. Here, we must make a distinction: A linear operator Φ on $\mathcal{M}_N(\mathbb{C})$ is *Hermitian* if and only if $\Phi(A^*) = (\Phi(A))^*$ for all $A \in \mathcal{M}_N(\mathbb{C})$. This is the only sense in which we shall use this term.

1.2. The problems considered

It is assumed that the reader is familiar with the notion of *completely positive* (CP) maps that was introduced by Stinespring [13], and have been much-studied since then. A concise account containing all that is needed here can be found in the early chapters of [12] or in [14]. By a quantum Markov semigroup, we mean a semigroup $\{\mathscr{P}_t\}_{t\geq 0}$ of linear operators on $\mathcal{M}_N(\mathbb{C})$ such that each $\mathscr{P}_t$ is completely positive and satisfies $\mathscr{P}_t(\mathbf{1}) = \mathbf{1}$. A map Φ on $\mathcal{M}_N(\mathbb{C})$ is *unital* in case $\Phi(\mathbf{1}) = \mathbf{1}$. Thus, when $\{\mathscr{P}_t\}_{t\geq 0}$ is a QMS, each $\mathscr{P}_t$ is unital, but unital CP maps are of wider interest in mathematical physics, and in this context are often referred to as *quantum operations*. The generator of a QMS $\{\mathscr{P}_t\}_{t\geq 0}$ is the operator $\mathscr{L}$ defined by

$$\mathscr{L} := \lim_{t\to 0} \frac{1}{t}(\mathscr{P}_t - I) \ .$$

Note that $\mathscr{L}\mathbf{1} = 0$, and $\mathscr{P}_t = e^{t\mathscr{L}}$.

We are interested here in CP maps and quantum Markov semigroups (QMS) and their generators that are self-adjoint with respect to the inner product $\langle\cdot,\cdot\rangle_m$ for some $m \in \mathcal{P}[0,1]$ and some $\sigma \in \mathfrak{S}_+$. The structure of the set of QMS generators that are self-adjoint with respect to the GNS and KMS inner products has been studied by mathematical physicists, but apart from these cases, not much is known.

1.2 Definition. For $m \in \mathcal{P}[0,1]$, let $\mathcal{H}_m$ denote the Hilbert space obtained by equipping $\mathcal{M}_N(\mathbb{C})$ with the inner product $\langle\cdot,\cdot\rangle_m$. Let CP_m denote the set of CP maps Φ on $\mathcal{M}_N(\mathbb{C})$ that are self-adjoint on $\mathcal{H}_m$, and let $CP_m(\mathbf{1})$ denote the subset of CP_m consisting of unital maps. Finally, let QMS_m denote the set of QMS generators that are self-adjoint on $\mathcal{H}_m$. We write CP to denote the set of all CP maps (without any particular self-adjointness requirement). Likewise, we write $CP(\mathbf{1})$ to denote the set of all CP unital maps and QMS to denote the set of all QMS generators.

As is well-known, both CP and QMS are convex cones. For CP this is obvious. If $\mathscr{L}_1$ and $\mathscr{L}_2$ are two generators of completely positive semigroups, then

$$e^{t(\mathscr{L}_1+\mathscr{L}_2)} = \lim_{k\to\infty} (e^{(t/k)\mathscr{L}_1} e^{(t/k)\mathscr{L}_2})^k \tag{1.12}$$

is completely positive, and hence the set of generators of completely positive semigroups is closed under addition, and also evidently under multiplication by non-negative real numbers. Since if $\mathscr{L}_j\mathbf{1} = 0$ for $j = 1, 2$, then $(\mathscr{L}_1+\mathscr{L}_2)\mathbf{1} = 0$, it follows easily that the set of all QMS semigroup generators is a convex cone. However, it is not a pointed cone: Let $H \in \mathcal{M}_N(\mathbb{C})$ be self-adjoint, and define $\mathscr{L}(A) = i[H, A]$. Then $e^{t\mathscr{L}}(A) = e^{itH}Ae^{-itH}$ is a QMS, and evidently both $\mathscr{L}$ and $-\mathscr{L}$ are QMS generators.

By a theorem of Lindblad [10] and Gorini, Kossakowski and Sudarshan [8], every QMS generator $\mathscr{L}$ on $\mathcal{M}_N(\mathbb{C})$ is of the form

$$\mathscr{L}(A) = (G^*A + AG) + \Phi(A) \tag{1.13}$$

where Φ is completely positive. Since $\mathscr{L}\mathbf{1} = 0$, $G^* + G = -\Phi(\mathbf{1})$. If we define $K := \frac{1}{2i}(G - G^*)$, then we can rewrite (1.13) as

$$\mathscr{L}(A) = \Phi(A) - \frac{1}{2}(\Phi(\mathbf{1})A + A\Phi(\mathbf{1})) - i[K, A] \ . \tag{1.14}$$

However, Φ and K are not uniquely determined by $\mathscr{L}$, and it is possible for $\mathscr{L}$ to be self-adjoint on $\mathcal{H}_m$ while Φ is not, and *vice-versa*. Hence the problem of determining the structure of CP_m is not the same as the problem of determining the structure of QMS_m.

There is a natural order relation on CP (without any requirement of self-adjointness), that was investigated by Arveson in [2]. He worked in the general context of CP maps from a C^* algebra $\mathscr{A}$ into $\mathcal{B}(\mathcal{H})$, the bounded operators on a Hilbert space $\mathcal{H}$. If Φ and Ψ are two such CP maps, we write $\Phi \geq \Psi$ in case $\Phi - \Psi$ is CP. An element Φ is called *extreme* in case whenever $\Psi \in CP$ and $\Phi \geq t\Psi$ for some $t > 0$, then Ψ is a multiple of Φ. Arveson also considered the set $CP(\mathbf{1})$ of unital CP maps. An element $\Phi \in CP(\mathbf{1})$ is extreme if whenever for some $0 < t < 1$ and $\Psi_1, \Psi_2 \in CP(\mathbf{1})$, $\Phi = t\Psi_1 + (1-t)\Psi_2$, $\Psi_1 = \Psi_2 = \Phi$. Equivalently, whenever $\Phi \geq t\Psi$ for some $0 < t < 1$ and $\Psi \in CP(\mathbf{1})$, then $\Psi = \Phi$.

For all $\Phi \in CP$, Arveson's Radon-Nikodym Theorem gives an explicit description of the set $\{\Psi \in CP \ : \ \Phi - \Psi \geq 0\}$. Using this, he proved a characterization of the extreme points of $CP(\mathbf{1})$. Later, Choi [5] gave a simplified treatment of Arveson's result in the case of matrix algebras. Every CP map on $M_N(\mathbb{C})$ has a Kraus representation [9]: There is a set $\{V_1, \dots, V_M\} \subset \mathcal{M}_N(\mathbb{C})$ such that for all $A \in \mathcal{M}_N(\mathbb{C})$,

$$\Phi(A) = \sum_{j=1}^{M} V_j^* A V_j \ , \tag{1.15}$$

and one may always take such a representation in which $\{V_1, \dots, V_M\}$ is linearly independent; such a Kraus representation is *minimal*. There is a close relation between minimal Kraus representations and minimal Stinespring representations that is recalled in an appendix. If (1.15) is *any* Kraus representation of Φ, then Φ is unital if and only if $\sum_{j=1}^{M} V_j^* V_j = \mathbf{1}$, and Choi's matricial version [5] of Arveson's theorem on extremality is that if (1.15) is a minimal Kraus representation, Φ is extremal in $CP(\mathbf{1})$ if and only if $\{V_i^* V_j \ : \ 1 \leq i, j \leq M\}$ is linearly independent.

While necessary and sufficient conditions for a QMS generator to be self-adjoint for the GNS or KMS inner products have been proved by Alicki [1] and Fagnola and Umanita [6,7], little appears to be known about the order structure and extreme points for CP_m, $CP_m(\mathbf{1})$ and QMS_m. Even for the case of the GNS or KMS inner products, there is more to say.

For the KMS inner product, let $CP_{KMS} := CP_{\delta_{1/2}}$. We prove the following results:

1.3 Theorem. *Let $\mathfrak{K}$ be the real vector space consisting of all $V \in \mathcal{M}_N(\mathbb{C})$ such that $\Delta^{-1/2}V = V^*$. The extremal elements Φ of CP_{KMS} are precisely the elements of the form*

$$\Phi(A) = V^*AV \ , \qquad V \in \mathfrak{K} \ . \tag{1.16}$$

Every map in CP_{KMS} is a positive linear combination of at most N^2 such maps.

1.4 Theorem. *Let Φ and Ψ be two CP maps that are KMS self-adjoint. Let $\Phi(A) = \sum_{j=1}^M V_j^*AV_j$ be a minimal Kraus representation of Φ with each $V_j \in \mathfrak{K}$. Then $\Phi - \Psi$ is CP if and only if there exists a real $M \times M$ matrix T such that $0 \le T \le \mathbf{1}$ and*

$$\Psi(A) = \sum_{i,j=1}^{M} T_{i,j}V_i^*AV_j \ . \tag{1.17}$$

1.5 Theorem. *Let Φ be a unital CP map that is KMS self-adjoint and let $\Phi(A) = \sum_{j=1}^M V_j^*AV_j$ be a minimal Kraus representation of Φ with $V_j \in \mathfrak{K}$ for each j. Then Φ is an extreme point of the set of unital CP maps that are KMS self-adjoint if and only if*

$$\{V_i^*V_j + V_j^*V_i \ : \ 1 \le i \le j \le M\} \tag{1.18}$$

is linearly independent over the real numbers.

Theorem 1.4 is an analog of Arveson's Radon-Nikodym Theorem for CP maps in the context of KMS self-adjointness. The matrix algebra version of Arveson's theorem states that if (1.15) is a minimal Kraus representation of a CP map Φ, and Ψ is another CP map, then $\Phi - \Psi$ is CP if and only if there is a complex $M \times M$ matrix T, $0 \le T \le \mathbf{1}$ such that Ψ is given by (1.17). The restriction that both Φ and Ψ are self-adjoint on $\mathcal{H}_{KMS}$ results in the further requirements that V_j belongs to the real vector space $\mathfrak{K}$ for each j, and that T is real. The matricial version of Arveson's theorem is proved in an appendix.

For every $m \in \mathcal{P}[0,1]$, there is a natural order on QMS_m. While QMS is not a pointed cone, QMS_m is always a pointed cone: We prove:

1.6 Theorem. *For any $m \in \mathcal{P}[0,1]$, if $\Phi \in QMS_m$ and $-\Phi \in QMS_m$, then $\Phi = 0$.*

For $\mathscr{L}_1, \mathscr{L}_2 \in QMS_m$, we define $\mathscr{L}_1 \ge \mathscr{L}_2$ to mean that $\mathscr{L}_1 - \mathscr{L}_2 \in QMS_m$. By Theorem 1.6, it follows that if $\mathscr{L}_1 \ge \mathscr{L}_2$ and $\mathscr{L}_2 \ge \mathscr{L}_1$, then $\mathscr{L}_1 = \mathscr{L}_2$. We then define an element $\mathscr{L} \in QMS_m$ to be *extremal* in case whenever $\widetilde{\mathscr{L}} \in QMS_m$ satisfies $\mathscr{L} \ge t\widetilde{\mathscr{L}}$ for some $t > 0$, $\widetilde{\mathscr{L}}$ is a non-zero multiple of $\mathscr{L}$.

The special feature of self-adjointness on $\mathcal{H}_m$ for $m = \delta_s$, and $s \in [0,1]$ that greatly simplifies the task of studying QMS_m in these cases is that there is an orthogonal

decomposition of $\widehat{\mathfrak{H}}$ into two subspaces, each of which is invariant under the operation of taking the adjoint on $\mathcal{H}_m$:

1.7 Definition. Define $\widehat{\mathfrak{H}}_{\mathcal{S}}$ to be the subspace of $\widehat{\mathfrak{H}}$ consisting of all operators Φ of the form

$$\Phi(A) = XA + AY \tag{1.19}$$

for some $X, Y \in \mathcal{M}_N(\mathbb{C})$.

We shall prove:

1.8 Lemma. *For each $s \in [0,1]$, both $\widehat{\mathfrak{H}}_{\mathcal{S}}$ and $\widehat{\mathfrak{H}}_{\mathcal{S}}^{\perp}$ are invariant under the operation of taking the adjoint with respect to the inner product $\langle \cdot, \cdot \rangle_{\delta_s}$. Moreover, if $\{V_1, \dots, V_M\}$ is linearly independent in $\mathcal{M}_N(\mathbb{C})$, the map $A \mapsto \sum_{j=1}^{M} V_j^* A V_j$ belongs to $\widehat{\mathfrak{H}}_{\mathcal{S}}^{\perp}$ if and only if $\mathrm{Tr}[V_j] = 0$ for each j.*

(Of course, once the invariance of one subspace is shown, the invariance of the other follows.)

Now consider any QMS generator $\mathscr{L}$. By the *LGKS* Theorem [10,8] recalled earlier in the introduction, $\mathscr{L}$ has the form

$$\mathscr{L}(A) = (G^*A + AG) + \Psi(A) \tag{1.20}$$

where Ψ is CP. Let

$$\Psi(A) = \sum_{j=1}^{M} V_j^* A V_j$$

be a minimal Kraus representation of Ψ. Replacing each V_j by $V_j - \mathrm{Tr}[V_j]\mathbf{1}$, and absorbing the difference into G, we may assume that $\mathrm{Tr}[V_j] = 0$ for each j. By Lemma 1.8, we then have $\Psi \in \widehat{\mathfrak{H}}_{\mathcal{S}}^{\perp}$. Furthermore, adding a purely imaginary multiple of $\mathbf{1}$ to G does not change $\mathscr{L}$, and hence we may also assume without loss of generality that $\mathrm{Tr}[G] \in \mathbb{R}$. Thus, making these choices for G and Ψ, (1.20) gives the decomposition of $\mathscr{L}$ into its components in $\widehat{\mathfrak{H}}_{\mathcal{S}}$ and $\widehat{\mathfrak{H}}_{\mathcal{S}}^{\perp}$. Then by Lemma 1.8, if $\mathscr{L}$ is self-adjoint on $\mathcal{H}_{\delta_s}$, each of these pieces must be *individually* self-adjoint on $\mathcal{H}_{\delta_s}$. For example, for $s = 1/2$, corresponding to the KMS inner product, Theorem 1.3 gives the necessary and sufficient conditions for Ψ to be self-adjoint, and then an easy computation shows that $A \mapsto G^*A + AG$ is self-adjoint on $\mathcal{H}_{KMS}$ if and only if $\Delta^{-1/2} G = G^*$, where we have taken, without loss of generality, $\mathrm{Tr}[G] \in \mathbb{R}$.

This brings us to a result of Fagnola and Umanita [6, Theorem 37]: Let $\mathscr{L} \in QMS$ be given in the form

$$\mathscr{L}(A) = G^*A + AG + \sum_{j=1}^{M} W_j^* A W_j$$

where $\mathrm{Tr}[G] \in \mathbb{R}$, $\{W_1, \dots, W_M\}$ is linearly independent, and for each j, $\mathrm{Tr}[W_j] = 0$. Then $\mathscr{L}$ is self-adjoint on $\mathcal{H}_{KMS}$ is and only if
(i) $\Delta^{-1/2} G = G^*$
(ii) There is an $M \times M$ unitary matrix $\widetilde{U}$ such that for each j, $\Delta^{-1/2} W_j = \sum_{k=1}^{M} \widetilde{U}_{j,k} W_k^*$.

We have already explained how condition *(i)* follows from Lemma 1.8 apart from the simple computation that will be provided below. As for *(ii)*, let $\Psi(A) = \sum_{j=1}^{M} W_j^* A W_j$. By Lemma 1.8, this must be self-adjoint on $\mathcal{H}_{KMS}$ and then by Theorem 1.3 there is another minimal Kraus representation $\Psi(A) = \sum_{j=1}^{M} V_j^* A V_j$, necessarily with the same M, such that $\Delta^{-1/2} V_j = V_j^*$. By the unitary equivalence of minimal Kraus representations (see the appendix), there is an $M \times M$ unitary matrix such that for each j, $W_j = \sum_{k=1}^{M} U_{j,k} V_k$ and hence

$$\Delta^{-1/2} W_j = \sum_{k=1}^{M} U_{j,k} \Delta^{-1/2} V_k = \sum_{k=1}^{M} U_{j,k} V_k^* = \sum_{k,\ell=1}^{M} U_{j,k} U_{\ell,k} W_k^* = \sum_{\ell=1}^{M} (UU^T)_{j,\ell} W_k^*$$

where U^T denotes the transpose of U, and of course $\widetilde{U} := UU^T$ is unitary.

Conversely, suppose that *(ii)* is satisfied. Let U be another unitary to be chosen below. Then for each ℓ,

$$\Delta^{-1/2} \left(\sum_{j=1}^{M} U_{\ell,j} W_j \right) = \sum_{j,k=1}^{M} U_{\ell,j} \widetilde{U}_{j,k} W_k^* \ ,$$

and thus if we choose U so that $\overline{U} = U\widetilde{U}$, we may define $V_j = \sum_{k=1}^{M} U_{j,k} W_k$, $\Psi(A) = \sum_{j=1}^{M} V_j^* A V_j$ and for each j, $\Delta^{-1/2} V_j = V_j^*$ and $\mathrm{Tr}[V_j] = 0$. It is easy to find such U: Choose an orthonormal basis in which $\widetilde{U}$ is diagonal with jth diagonal entry $e^{i\theta_j}$. We may take U to be diagonal in this same basis with jth diagonal entry $e^{-i\theta_j/2}$.

The result of Fagnola and Umanita allows one to check whether or not any given QMS generator is self-adjoint on $\mathcal{H}_{KMS}$. However, it does not provide a parameterization of QMS_{KMS}, the cone of QMS generators that are self-adjoint on $\mathcal{H}_{KMS}$, nor can one readily read off the set of extreme points from their result; there are compatibility conditions relating G and $\{W_1, \dots, W_M\}$. The following result provides this and other additional information:

1.9 Theorem. *There is a one-to-one correspondence between elements $\mathscr{L}$ of QMS_{KMS} and CP maps $\Psi \in \widehat{\mathfrak{H}}_{\mathcal{S}}^{\perp}$ that are self-adjoint on $\mathcal{H}_{KMS}$. The correspondence identifies Ψ with $\mathscr{L}_\Psi$ where*

$$\mathscr{L}_\Psi(A) = G^*A + AG + \Psi(A) \tag{1.21}$$

where $G = H + iK$, H and K self-adjoint and given by

$$H := \tfrac{1}{2}\Psi(\mathbf{1}) \tag{1.22}$$

and

$$K := \frac{1}{i}\int_0^\infty e^{-t\sigma^{1/2}}(\sigma^{1/2}H - H\sigma^{1/2})e^{-t\sigma^{1/2}}\mathrm{d}t\ . \tag{1.23}$$

Furthermore, for all $\mathscr{L}_{\Psi_1}, \mathscr{L}_{\Psi_2} \in QMS_{KMS}$, $\mathscr{L}_{\Psi_1} - \mathscr{L}_{\Psi_2} \in QMS$ if and only if $\Psi_1 - \Psi_2 \in CP$; i.e., $\mathscr{L}_{\Psi_1} \geq \mathscr{L}_{\Psi_2}$ if and only if $\Psi_1 \geq \Psi_2$, and the extreme points of QMS_{KMS} are precisely the generators of the form

$$\mathscr{L}(A) := G^*A + AG + V^*AV$$

where $\Delta^{-1/2}V = V^*$ and where $G = H + iK$ is given by (1.22) and (1.23) for $\Psi(A) = V^*AV$.

1.10 Remark. It is easy to see that K defined by (1.23) satisfies $\mathrm{Tr}[K] = 0$, so that $\mathrm{Tr}[G] \in \mathbb{R}$.

We also prove analogous results for self-adjointness with respect to the inner products on $\mathcal{H}_{\delta_s}$ for all $s \neq 1/2$. This includes the GNS case, and in fact it is well known that for $s \neq 1/2$, any Hermitian operator Φ is self-adjoint on $\mathcal{H}_{\delta_s}$ for *all* $s \neq 1/2$ if and only if it is self-adjoint on $\mathcal{H}_{GNS} = \mathcal{H}_{\delta_0}$. It follows that Hermitian operators Φ that are self-adjoint on $\mathcal{H}_{GNS}$ are *universally self-adjoint* – they are self-adjoint on $\mathcal{H}_m$ for all m. The results specifying extreme points, e.g., of the set of GNS self-adjoint unital CP maps, etc., are new, as is the theorem giving necessary conditions for $\Phi_1 - \Phi_2 \in CP$ when Φ_1 and Φ_2 are CP and self-adjoint on $\mathcal{H}_{GNS}$, while the structure of QMS_{GNS} was worked out by Alicki [1].

We turn next to the BKM inner product, whose investigation is motived in part by [4, Theorem 2.9]. It is much more difficult to prove analogs of the theorems proved here for the KMS and GNS inner product, in part because $\widetilde{\mathfrak{H}}_S^{\perp}$ is not invariant under the operation of taking the BKM adjoint. However, the BKM case shares one very nice feature with the KMS case; in both cases $\mathcal{M}_m^{-1}$ is CP. Using this, we construct and study a one-to-one map from CP_{KMS} into CP_{BKM}. This map is unfortunately not surjective, but it does also take unital maps to unital maps, and so it gives us a large class of quantum operations that are self-adjoint on $\mathcal{H}_{BKM}$.

Finally, we study operators that are *evenly self-adjoint*, by which we mean self-adjoint on $\mathcal{H}_m$ for all even m. The class of evenly self-adjoint QMS generators is strictly larger than the class of GNS self-adjoint QMS generators, but also strictly smaller than the set of QMS generators that are BKM or KMS self-adjoint.

2. Background material

We recall some useful tools. It is convenient to index orthonormal bases of $\mathfrak{H}$ by ordered pairs $(i,j) \in \{1,\dots N\} \times \{1,\dots N\} =: \mathcal{J}_N$. We use lower case Greek letters to denote elements of the index set. For $\alpha = (i,j) \in \mathcal{J}_N$, $\alpha' := (j,i)$.

For $F, G \in \mathcal{M}_N(\mathbb{C})$, define the operator $\#(F \otimes G)$ on $\mathfrak{H}$ by

$$\#(F \otimes G)X := FXG \ . \tag{2.1}$$

Simple computations show that

$$\langle \#(F_1 \otimes G_1), \#(F_2 \otimes G_2)\rangle_{\widehat{\mathfrak{H}}} = \langle F_1, F_2\rangle_{\mathfrak{H}} \langle G_1, G_2\rangle_{\mathfrak{H}} \ . \tag{2.2}$$

Hence, if $\{F_\alpha\}_{\alpha\in\mathcal{J}_N}$ and $\{G_\alpha\}_{\alpha\in\mathcal{J}_N}$ are two orthonormal bases of $\mathfrak{H}$, $\{\#(F_\alpha \otimes G_\beta)\}_{\alpha,\beta\in\mathcal{J}_N}$ is an orthonormal basis of $\widehat{\mathfrak{H}}$.

Now fix any orthonormal basis $\{F_\alpha\}_{\alpha\in\mathcal{J}_N}$ of $\mathfrak{H}$. Then $\{F_\alpha^*\}_{\alpha\in\mathcal{J}_N}$ is also an orthonormal basis of $\mathfrak{H}$, and hence $\{\#(F_\alpha^* \otimes F_\beta)\}_{\alpha,\beta\in\mathcal{J}_N}$ is an orthonormal basis of $\widehat{\mathfrak{H}}$. Thus, every linear operator Φ on $\mathfrak{H}$ has an expansion

$$\Phi = \sum_{\alpha,\beta\in\mathcal{J}_N} (c_\Phi)_{\alpha,\beta} \#(F_\alpha^* \otimes F_\beta) \ , \tag{2.3}$$

where

$$(c_\Phi)_{\alpha,\beta} = \langle \#(F_\alpha^* \otimes F_\beta), \Phi\rangle_{\widehat{\mathfrak{H}}} \ . \tag{2.4}$$

In particular, the coefficients $(c_\Phi)_{\alpha,\beta}$ are uniquely determined. The following definition is from [8]; see the Appendix of [3] for more information.

2.1 Definition *(Characteristic matrix).* Given a linear operator Φ on $\mathfrak{H}$, and an orthonormal basis $\{F_\alpha\}_{\alpha\in\mathcal{J}_N}$ of $\mathfrak{H}$, its *characteristic matrix* for this orthonormal basis is the $N^2 \times N^2$ matrix C_Φ whose (α,β)th entry is $(c_\Phi)_{\alpha,\beta}$ as specified in (2.4).

2.2 Remark. An easy computation shows the following: Let Φ be a linear operator on $\mathfrak{H}$. Let $\{F_\alpha\}$ and $\{\widetilde{F}_\alpha\}$ be two orthonormal bases of $\mathfrak{H}$. Let C_Φ be the characteristic matrix of Φ with respect to $\{F_\alpha\}$, and let $\widetilde{C}_\Phi$ be the characteristic matrix of Φ with respect to $\{\widetilde{F}_\alpha\}$. Let U be the $N^2 \times N^2$ unitary matrix such that $\widetilde{F}_\alpha = \sum_\beta U_{\alpha,\beta} F_\beta$. Then $\tilde{C}_\Phi = UC_\Phi U^*$.

2.3 Lemma *(See [8]). A linear operator Φ on $\mathfrak{H}$ is Hermitian if and only if C_Φ, for any orthonormal basis $\{F_\alpha\}_{\alpha\in\mathcal{J}_N}$, is self-adjoint.*

Proof. We compute

$$(\Phi(A^*))^* := \left(\sum_{\alpha,\beta\in\mathcal{J}_N} (c_\Phi)_{\alpha,\beta} F_\alpha^* A^* F_\beta\right)^* = \sum_{\alpha,\beta\in\mathcal{J}_N} \overline{(c_\Phi)_{\alpha,\beta}} F_\beta^* A^* F_\alpha$$
$$= \sum_{\alpha,\beta\in\mathcal{J}_N} \overline{(c_\Phi)_{\beta,\alpha}} F_\alpha^* A^* F_\beta \ .$$

By the uniqueness of the coefficients, Φ is Hermitian if and only if $(c_\Phi)_{\alpha,\beta} = \overline{(c_\Phi)_{\beta,\alpha}}$ for all α, β. □

The following lemma is a variant of Choi's Theorem [5]; see [8] for this version.

2.4 Lemma. *A linear operator Φ on $\mathcal{M}_N(\mathbb{C})$ is completely positive if and only if for every orthonormal basis $\{F_\alpha\}_{\alpha\in\mathcal{J}_N}$ of $\mathfrak{H}$, the corresponding characteristic matrix C_Φ is positive semi-definite.*

Proof. The right side of (2.4) can be computed using the matrix unit basis to compute the trace:

$$(c_\Phi)_{\alpha,\beta} = \langle \#(F_\alpha^* \otimes F_\beta), \Phi\rangle_{\hat{\mathfrak{H}}} = \frac{1}{N^2} \sum_{1\le k,\ell\le N} \mathrm{Tr}[E_{k,\ell}^* F_\alpha \Phi(E_{k,\ell}) F_\beta^*]$$

Let $(z_1, \dots, z_{N^2}) \in \mathbb{C}^{N^2}$ and define $G := \sum_{\alpha\in\mathcal{J}_N} z_\alpha F_\alpha^*$. Then

$$\sum_{\alpha,\beta} \overline{z}_\alpha (c_\Phi)_{\alpha,\beta} z_\beta = \frac{1}{N^2} \sum_{1\le k,\ell\le N} \mathrm{Tr}[E_{\ell,k} G^* \Phi(E_{k,\ell}) G] \ . \tag{2.5}$$

Let $[E_{i,j}]$ denote the block matrix whose i,jth entry is $E_{i,j}$. Then it is easy to see that $N^{-1/2}[E_{i,j}]$ is an orthogonal projection, and in particular, positive. Now suppose that Φ is completely positive. Then the block matrix $[G^*\Phi(E_{i,j})G]$ whose i,jth entry is $G^*\Phi(E_{i,j})G$ is positive. The right side of (2.5) is then the trace (on the direct sum of N copies of $\mathbb{C}^N$) of the product of positive $N^2 \times N^2$ matrices, and as such it is positive. Thus, whenever Φ is completely positive, C_Φ is positive semi-definite.

On the other hand, suppose that C_Φ is positive semi-definite. Let Λ be a diagonal matrix whose diagonal entries are the eigenvalues of C_Φ, and let U be a unitary such that $C_\Phi = U^*\Lambda U$. Then by (2.3), for any $X \in \mathfrak{H}$,

$$\Phi(X) = \sum_{\alpha,\beta,\gamma\in\mathcal{J}_N} U_{\alpha,\gamma}^* \lambda_k U_{\gamma,\beta} F_\alpha^* X F_\beta = \sum_{\gamma\in\mathcal{J}_N} V_\gamma^* X V_\gamma \ ,$$

where $V_\gamma := \sqrt{\lambda_\gamma} \sum_{\alpha\in\mathcal{J}_N} U_{\gamma,\alpha} F_\alpha$. This shows that whenever C_Φ is positive semi-definite, Φ is completely positive, and provides a Kraus representation of it. □

So far, we have not required any special properties of the orthonormal bases $\{F_\alpha\}_{\alpha\in\mathcal{J}_N}$ of $\mathfrak{H}$ that we used. Going forward, it will be necessary to choose bases that have several useful properties:

2.5 Definition *(symmetric, unital and matrix unit bases).* An orthonormal basis $\{F_\alpha\}_{\alpha\in\mathcal{J}_N}$ of $\mathfrak{H}$ is *symmetric* in case

$$\text{for all} \quad \alpha \in \mathcal{J}_N \ , \quad F_\alpha^* = F_{\alpha'} \ . \tag{2.6}$$

It is *unital* in case it is symmetric and moreover

$$F_{(1,1)} = \mathbf{1} \ . \tag{2.7}$$

It is the *matrix unit* basis corresponding to an orthonormal basis $\{u_1, \dots, u_N\}$ of $\mathbb{C}^N$ in case

$$F_{(i,j)} = \sqrt{N}|u_i\rangle\langle u_j| \ . \tag{2.8}$$

Note that a matrix unit basis is symmetric.

One reason unital bases are useful is the following: the characteristic matrix C_I of the identity transformation $I(A) = A$ in a unital basis $\{F_\alpha\}_{\alpha\in\mathcal{J}_N}$ has only one nonzero entry, a 1 in the upper left corner. Indeed, for any A, the expansion of $I(A)$ in the form $\sum_{\alpha\beta} \#(F_\alpha^* \otimes F_\beta)(A) = \sum_{\alpha\beta}(c_I)_{\alpha,\beta}F_\alpha^* A F_\beta$ reads simply $\mathbf{1}^* A \mathbf{1} = F_{(1,1)}^* A F_{(1,1)}$. This fact will be used later.

2.6 Remark. When studying self-adjointness with respect to the various inner products we have introduced, the following bases will be particularly useful: Let $\sigma \in \mathfrak{S}_+(\mathcal{A})$, and let $\{u_1, \dots, u_N\}$ be an orthonormal basis of $\mathbb{C}^N$ consisting of eigenvectors of σ:

$$\sigma u_j = \lambda_j u_j \ , \quad j = 1, \dots, N \ .$$

The associated matrix unit basis is then given by

$$E_{(i,j)} = \sqrt{N}|u_i\rangle\langle u_j| \ . \tag{2.9}$$

We can then construct a unital basis from this as follows: Let v_1 be the unit vector $N^{-1/2}(1, \dots, 1) \in \mathbb{C}^N$ each of whose entries $(v_1)_k = N^{-1/2}$. Let $e_1 = (1, 0, \dots, 0)$ be the unit vector in $\mathbb{C}^N$ whose first entry is 1. Define

$$u := \frac{1}{\|v_1 - e_1\|}(v_1 - e_1) \qquad \text{and} \qquad V := \mathbf{1} - 2|u\rangle\langle u| \ .$$

Then it is evident that V is a self-adjoint real unitary matrix, and that $Ve_1 = v_1$. (V is the Householder reflection of e_1 onto v_1). Since Ve_1 is the first column of V, the first

column of V is v_1, and then since V is symmetric, the first row of V is also v_1. One readily finds that

$$\sqrt{N}V_{i,j} = \begin{cases} 1 & i = 1 \text{ or } j = 1 \\ \frac{N-2}{\sqrt{N}-1} - 1 & i = j \geq 2 \\ \frac{-1}{\sqrt{N}-1} & \text{otherwise} \end{cases} \tag{2.10}$$

Let U be the $N^2 \times N^2$ unitary matrix whose lower right $(N^2 - N) \times (N^2 - N)$ block is the identity, and whose upper left $N \times N$ block is V. That is, for $N = 2$,

$$U = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} . \tag{2.11}$$

Then using this unitary U, we define

$$F_\alpha := \sum_\beta U_{\alpha,\beta} E_\beta \ . \tag{2.12}$$

Then $\{F_\alpha\}_{\alpha \in \mathcal{J}_N}$ is a unital basis; in particular $F_{(1,1)} = \mathbf{1}$.

We are now ready to recall the characterization of QMS generators. Again, the definition is due to [8].

2.7 Definition *(Reduced characteristic matrix).* Let $\mathscr{L}$ be a Hermitian operator on $\mathfrak{H}$ such that $\mathscr{L}\mathbf{1} = 0$, and let $\{F_\alpha\}_{\alpha \in \mathcal{J}_N}$ be a unital orthonormal basis. Let $C_{\mathscr{L}}$ be the characteristic matrix of $\mathscr{L}$ with respect to this basis. The *reduced characteristic matrix* $R_{\mathscr{L}}$ of $\mathscr{L}$ is the $(N^2-1)\times(N^2-1)$ matrix obtained by deleting the first row and column of $C_{\mathscr{L}}$.

The point of this definition is the following, due to [8,11].

2.8 Lemma. *Let $\mathscr{L}$ be a Hermitian operator on $\mathfrak{H}$ such that $\mathscr{L}\mathbf{1} = 0$, and let $\{F_\alpha\}_{\alpha \in \mathcal{J}_N}$ be a unital orthonormal basis. Let $R_{\mathscr{L}}$ be the reduced characteristic matrix of $\mathscr{L}$ with respect to this basis. Then $\mathscr{L}$ is a QMS generator if and only if $R_{\mathscr{L}}$ is positive semi-definite.*

Proof. Suppose that $\mathscr{P}_t := e^{t\mathscr{L}}$ is completely positive for each $t > 0$. By the computation of the characteristic matrix C_I of the identity transformation I performed earlier, we know that its reduced characteristic matrix $R_I = 0$. Then since

$$R_{t^{-1}(\mathscr{P}_t - I)} = t^{-1} R_{\mathscr{P}_t} - t^{-1} R_I = t^{-1} R_{\mathscr{P}_t} \ ,$$

the reduced characteristic matrix of $t^{-1}(\mathscr{P}_t - I)$ coincides with the reduced characteristic matrix of $t^{-1}\mathscr{P}_t$, and by Lemma 2.4 this is positive. Taking the limit $t \to 0$, we conclude that the reduced characteristic matrix of $\mathscr{L}$ is positive.

Conversely, suppose that the reduced characteristic matrix of $\mathscr{L}$ is positive. Since $F_{(1,1)} = \mathbf{1}$,

$$\mathscr{L}(A) = \sum_{\alpha,\beta} (c_{\mathscr{L}})_{\alpha,\beta} F_\alpha^* A F_\beta = G^* A + AG + \sum_{\alpha,\beta} (r_{\mathscr{L}})_{\alpha,\beta} F_\alpha^* A F_\beta$$

where

$$G := \frac{1}{2}(c_{\mathscr{L}})_{(1,1),(1,1)} \mathbf{1} + \sum_\beta (c_{\mathscr{L}})_{(1,1),\beta} F_\beta \ .$$

By Lemma 2.4, if we define $\Psi(A) := \sum_{\alpha,\beta} (r_{\mathscr{L}})_{\alpha,\beta} F_\alpha^* A F_\beta$, then Ψ is completely positive. Defining $\Phi(A) := G^* A + AG$, we have $\mathscr{L} = \Phi + \Psi$, and then by the argument around (1.12), $e^{t\mathscr{L}}$ is completely positive for all $t > 0$. Finally, since $\mathscr{L}\mathbf{1} = 0$, $e^{t\mathscr{L}}$ is a QMS. □

We are also interested in characterizing the characteristic matrices of operators Φ in $\mathfrak{H}$ for which $\Phi\mathbf{1} = 0$, and, for some $\sigma \in \mathfrak{S}_+$, $\Phi^\dagger \sigma = 0$.

2.9 Lemma. *Let $\{E_\alpha\}$ be a matrix unit basis of $\mathfrak{H}$. Let Φ be an operator on $\mathfrak{H}$, and let C_Φ be its characteristic matrix with respect to $\{E_\alpha\}$. Then $\Phi(\mathbf{1}) = 0$ if and only if for each $1 \le k, \ell \le N$*

$$\sum_{j=1}^N (c_\Phi)_{(j,k),(j,\ell)} = 0 \ , \tag{2.13}$$

and $\Phi(\mathbf{1}) = \mathbf{1}$ if and only if (2.13) is satisfied for $k \neq \ell$, and for $1 \le k \le N$,

$$\sum_{j=1}^N (c_\Phi)_{(j,k),(j,k)} = \frac{1}{N} \ . \tag{2.14}$$

Proof. We compute

$$\Phi(\mathbf{1}) = \sum_{\alpha,\beta} (c_\Phi)_{\alpha,\beta} E_\alpha^* \mathbf{1} E_\beta = \sum_{\alpha,\beta} (c_\Phi)_{\alpha,\beta} \delta_{\alpha_1,\beta_1} E_{\alpha_2,\beta_2} = \sum_{j,k,\ell} (c_\Phi)_{(j,k),(j,\ell)} E_{(k,\ell)} \ ,$$

from which (2.13) follows, and then (2.14) follows since $\mathbf{1} = \frac{1}{N} \sum_{k=1}^N E_{(k,k)}$. □

2.10 Lemma. *Let Φ be an Hermitian operator on $\mathfrak{H}$, and let C_Φ be its characteristic matrix with respect to a symmetric orthonormal basis $\{F_\alpha\}_{\alpha \in \mathcal{J}_N}$ of $\mathfrak{H}$. Then*

$$(\#(F_\alpha^* \otimes F_\beta))^\dagger = \#F_{\alpha'}^* \otimes F_{\beta'} \ , \tag{2.15}$$

and

$$(c_{\Phi^\dagger})_{\alpha,\beta} = (c_\Phi)_{\beta',\alpha'} \ . \tag{2.16}$$

Proof. We compute

$$\mathrm{Tr}[B^* \# (F_\alpha^* \otimes F_\beta)(A)] = \mathrm{Tr}[B^* F_\alpha^* A F_\beta] = \mathrm{Tr}[(F_\alpha B F_\beta^*)^* A] = \mathrm{Tr}[(F_{\alpha'}^* B F_{\beta'})^* A] \ ,$$

and this proves (2.15). Then since $\Phi = \sum_{\alpha,\beta} (c_\Phi)_{\alpha,\beta} \# (F_\alpha^* \otimes F_\beta)$ and since $\overline{(c_\Phi)_{\alpha,\beta}} = (c_\Phi)_{\beta,\alpha}$ by Lemma 2.3,

$$\Phi^\dagger = \sum_{\beta,\alpha} \overline{(c_\Phi)_{\alpha,\beta}} (\#(F_\alpha^* \otimes F_\beta))^\dagger \ .$$

Then by (2.15), (2.16) follows. □

The next lemma says that for $\Phi \in CP(\mathbf{1})$ or $\mathscr{L} \in QMS$, there is often exactly one $\sigma \in \mathfrak{S}_+$ with respect to which Φ or $\mathscr{L}$ can possibly be self-adjoint on $\mathcal{H}_m$ for that choice of σ.

2.11 Lemma. *Let Φ be a Hermitian operator that is self-adjoint on $\mathcal{H}_m$ where $\mathcal{H}_m$ is defined in terms of some $\sigma \in \mathfrak{S}_+$. If $\Phi(\mathbf{1}) = \mathbf{1}$, then $\Phi^\dagger(\sigma) = \sigma$, and if $\Phi(\mathbf{1}) = 0$, then $\Phi^\dagger(\sigma) = 0$. Hence if $\Phi \in CP(\mathbf{1})$ is such that 1 is a non-degenerate eigenvalue of Φ, then for any $m \in \mathcal{P}[0,1]$, there can be only one $\sigma \in \mathfrak{S}_+$ such that Φ is self-adjoint on $\mathcal{H}_m$. Likewise, if $\mathscr{L} \in QMS$ is such that 0 is a non-degenerate eigenvalue of $\mathscr{L}$, then for any $m \in \mathcal{P}[0,1]$, there can be only one $\sigma \in \mathfrak{S}_+$ such that $\mathscr{L}$ is self-adjoint on $\mathcal{H}_m$.*

Proof. For any Hermitian operator Φ in $\mathfrak{H}$, any $\sigma \in \mathfrak{S}_+$ and any $m \in \mathcal{P}[0,1]$ such that Φ is self-adjoint on $\mathcal{H}_m$, we compute that for all A,

$$\mathrm{Tr}[\Phi^\dagger(\sigma) A] = \mathrm{Tr}[\sigma \Phi(A)] = \langle \mathbf{1}, \Phi(A) \rangle_m = \langle \Phi(\mathbf{1}), A \rangle_m \ .$$

If $\Phi(\mathbf{1}) = \mathbf{1}$, we have $\mathrm{Tr}[\Phi^\dagger(\sigma) A] = \mathrm{Tr}[\sigma A]$ and since A is arbitrary $\Phi^\dagger(\sigma) = \sigma$. Likewise, if $\Phi(\mathbf{1}) = 0$, we have $\mathrm{Tr}[\Phi^\dagger(\sigma) A] = 0$ and since A is arbitrary $\Phi^\dagger(\sigma) = 0$. □

On account of this lemma, we will only rarely make the choice of σ explicit in our notation. In the next section we determine necessary and sufficient conditions for self-adjointness.

3. Characterization for self-adjointness with respect to $\langle \cdot, \cdot \rangle_m$

For $m \in \mathcal{P}[0,1]$, let $(\cdot,\cdot)_m$ denote the *m-weighted mean* of two nonnegative numbers x, y:

$$(x,y)_m = \int_0^1 x^s y^{1-s}\, \mathrm{d}m(s) \quad , \quad x,y \in \mathbb{R}_+ \ . \tag{3.1}$$

Note that for all $m \in \mathcal{P}[0,1]$,

$$\min\{x,y\} \leq (x,y)_m \leq \max\{x,y\} \qquad \text{and} \qquad (x,x)_m = x \quad \text{for all } x \in \mathbb{R}_+ \ . \tag{3.2}$$

For m even,

$$(x,y)_m = (y,x)_m \quad \text{for all } x,y \in \mathbb{R}_+ \ . \tag{3.3}$$

Otherwise define $\widehat{m}$ to be the reflection of m about 1/2; i.e., $\widehat{m}(U) = m(1-U)$. Then

$$(x,y)_m = (y,x)_{\widehat{m}} \quad \text{for all } x,y \in \mathbb{R}_+ \ . \tag{3.4}$$

3.1 Remark. For any even $m \in \mathcal{P}[0,1]$ and any $x,y \in \mathbb{R}_+$, $x \neq y$, we have

$$\sqrt{xy} = (x,y)_{\mathrm{KMS}} \leq (x,y)_m \ , \tag{3.5}$$

with equality if and only if $m = \delta_{1/2}$. Indeed, first use symmetry of m to rewrite

$$(x,y)_m = \frac{1}{2}\int_0^1 (x^s y^{1-s} + x^{1-s}y^s)\mathrm{d}m(s) \ . \tag{3.6}$$

Then

$$(x^s y^{1-s} + x^{1-s}y^s) - \sqrt{xy} = \frac{1}{2}(x^{s/2}y^{(1-s)/2} + x^{(1-s)/2}y^{s/2})^2 \ ,$$

and integrating against m,

$$(x,y)_m - (x,y)_{\mathrm{KMS}} = \frac{1}{2}\int_0^1 (x^{s/2}y^{(1-s)/2} - x^{(1-s)/2}y^{s/2})^2 \mathrm{d}m(s) \ ,$$

and for $x \neq y$, the integrand vanishes only for $s = \frac{1}{2}$.

For $m \in \mathcal{P}[0,1]$ let $\mathcal{M}_m$ be the linear transformation on $\mathfrak{H}$ defined in (1.2). Let $\{u_1, \ldots, u_N\}$ be a complete orthonormal basis of $\mathbb{C}^N$ consisting of eigenvectors of σ so that $\sigma u_j = \lambda_j u_j$ for each j. By hypothesis, each λ_j is strictly positive. Let $\{E_\alpha\}_{\alpha \in \mathcal{J}_N}$ be the associated matrix unit basis;

$$E_{(j,k)} := \sqrt{N}|u_j\rangle\langle u_k| \ . \tag{3.7}$$

Then

$$\mathcal{M}_m(E_{(j,k)}) = (\lambda_j, \lambda_k)_m E_{(j,k)} \ .$$

That is, $\mathcal{M}_m$ is diagonalized by the orthonormal basis of $\mathfrak{H}$ consisting of $\{\sqrt{N}E_{(j,k)}\}_{1\leq j,k\leq N}$. Since all of the eigenvalues are strictly positive, it follows that $\mathcal{M}$ is a positive, invertible operator on $\mathfrak{H}$, and the inverse is given by

$$\mathcal{M}_m^{-1}(E_{(j,k)}) = \frac{1}{(\lambda_j, \lambda_k)_m} E_{(j,k)} \ .$$

Since $E^*_{(j,k)} = E_{(k,j)}$, we also have, with $\widehat{m}$ denoting the reflection of m about $s = 1/2$,

$$\mathcal{M}_m(A^*) = (\mathcal{M}_{\widehat{m}}(A))^* \qquad \text{and} \qquad \mathcal{M}_m^{-1}(A^*) = (\mathcal{M}_{\widehat{m}}^{-1}(A))^* \tag{3.8}$$

In particular, if m is even, $\mathcal{M}_m$ and $\mathcal{M}_m^{-1}$ are Hermitian.

3.2 Lemma. *With respect to a matrix unit basis $\{E_\alpha\}_{\alpha\in\mathcal{J}_N}$ associated to σ, the characteristic matrices $C_{\mathcal{M}_m}$ and $C_{\mathcal{M}_m^{-1}}$ of $\mathcal{M}_m$ and $\mathcal{M}_m^{-1}$ are given by*

$$(c_{\mathcal{M}_m})_{\alpha,\beta} = (\alpha_1, \beta_1)_m \delta_{\alpha_1,\alpha_2}\delta_{\beta_1,\beta_2} \quad \text{and} \quad (c_{\mathcal{M}_m^{-1}})_{\alpha,\beta} = (\alpha_1, \beta_1)_m^{-1} \delta_{\alpha_1,\alpha_2}\delta_{\beta_1,\beta_2}. \tag{3.9}$$

Proof. We compute

$$\begin{aligned}
(c_{\mathcal{M}_m})_{\alpha,\beta} &= \frac{1}{N^2}\sum_{i,j} \mathrm{Tr}[(E^*_\alpha E_{(i,j)} E_\beta))^* \mathcal{M}_m(E_{(i,j)})] \\
&= \frac{1}{N^2}\sum_{i,j} (\lambda_i, \lambda_j)_m \mathrm{Tr}[(E^*_\alpha E_{(i,j)} E_\beta))^* E_{(i,j)}] \\
&= \frac{1}{N^2}\sum_{i,j} (\lambda_i, \lambda_j)_m \mathrm{Tr}[E^*_\beta E_{(j,i)} E_\alpha E_{(i,j)}] = \sum_{i,j} (\lambda_i, \lambda_j)_m \delta_{\beta_1,j}\delta_{\beta_2,j}\delta_{\alpha_1,i}\delta_{\alpha_2,i} \ ,
\end{aligned}$$

from which the first formula follows. The second follows in the same way. □

Hence, if we order the basis $\{E_\alpha\}_{\alpha\in\mathcal{J}_N}$ so that the first N unit vectors are

$$E_{(1,1)}, \ldots, E_{(N,N)}$$

in this order, then $C_{\mathcal{M}_m}$ and $C_{\mathcal{M}_m^{-1}}$ are both zero except in their upper left $N \times N$ blocks where the (i,j)th entries are $(\lambda_i, \lambda_j)_m$ and $(\lambda_i, \lambda_j)_m^{-1}$ respectively.

Now let A be a symmetric $N \times N$ matrix with positive entries. Then a necessary condition for A to be positive semi-definite is that for all i, j $A_{i,j} \leq \sqrt{A_{i,i}A_{j,j}}$. For $N = 2$, the condition is also sufficient, but it is easy to see that sufficiency fails already for $N = 3$.

However, combining the necessity with Remark 3.1, we see that $\mathcal{M}_m$ is never completely positive except in the KMS case, $m = \delta_{1/2}$, corresponding to the geometric mean. On the other hand, at least in the 2×2 case, $\mathcal{M}_m^{-1}$ is completely positive whenever m is even. There are important cases in which $\mathcal{M}_m^{-1}$ is completely positive in every dimension, including the KMS and BKM cases. We return to this later.

3.3 Definition. Let Φ be a linear transformation on $\mathcal{M}_N(\mathbb{C})$, and hence on $\mathcal{H}_m$ for each $m \in \mathcal{P}[0,1]$. Its adjoint with respect to the inner product $\langle \cdot, \cdot \rangle_m$ is denoted $\Phi^{*,m}$.

3.4 Lemma. *Let Φ be an Hermitian linear transformation on $\mathcal{M}_N(\mathbb{C})$ and let $m \in \mathcal{P}[0,1]$. Then*

$$\Phi^{*,m} = \mathcal{M}_m^{-1} \circ \Phi^\dagger \circ \mathcal{M}_m \ . \tag{3.10}$$

Proof. First recall that, since Φ is Hermitian, $\Phi^\dagger$ is Hermitian. To see this, note that

$$\begin{aligned} \mathrm{Tr}[(\Phi^\dagger(B^*))^* A] &= \mathrm{Tr}[B\Phi(A)] = \overline{\mathrm{Tr}[B^*(\Phi(A))^*]} = \overline{\mathrm{Tr}[B^*\Phi(A^*)]} \\ &= \overline{\mathrm{Tr}[(\Phi^\dagger B)^* A^*]} = \mathrm{Tr}[(\Phi^\dagger B)A] \ . \end{aligned}$$

Thus, $(\Phi^\dagger(B^*))^* = \Phi^\dagger(B)$ for all B.

We now compute

$$\begin{aligned} \langle B, \Phi(A)\rangle_m &= \mathrm{Tr}[B^* \mathcal{M}_m(\Phi(A))] = \mathrm{Tr}[(\mathcal{M}_m(B))^* \Phi(A)] \\ &= \mathrm{Tr}[(\Phi^\dagger(\mathcal{M}_m(B)))^* A] \\ &= \mathrm{Tr}[(\mathcal{M}_m^{-1}(\Phi^\dagger(\mathcal{M}_m(B))))^* \mathcal{M}_m(A)] \end{aligned}$$

Then (3.10) follows from (3.8). □

It follows that an Hermitian operator Φ is self-adjoint on $\mathcal{H}_m$ if and only if

$$\mathcal{M}_m \circ \Phi = \Phi^\dagger \circ \mathcal{M}_m \ . \tag{3.11}$$

3.5 Lemma. *Let $\{E_\alpha\}$ be the orthonormal basis of $\mathfrak{H}$ specified in (3.7). Then for all $m \in \mathcal{P}[0,1]$,*

$$\#(E_\alpha^* \otimes E_\beta) \circ \mathcal{M}_m = (\lambda_{\alpha_1}, \lambda_{\beta_1})_m \#(E_\alpha^* \otimes E_\beta) \tag{3.12}$$

and

$$\mathcal{M}_m \circ \#(E_\alpha^* \otimes E_\beta) = (\lambda_{\alpha_2}, \lambda_{\beta_2})_m \#(E_\alpha^* \otimes E_\beta) \tag{3.13}$$

Proof. We compute

$$E_\alpha^* \mathcal{M}_m(A) E_\beta = \int_0^1 E_\alpha^* \sigma^{1-s} A \sigma^s E_\beta \mathrm{d}m = (\lambda_{\alpha_1}, \lambda_{\beta_1})_m E_\alpha^* A E_\beta \ ,$$

and this proves (3.12).

Next, since $\mathcal{M}_m^\dagger = \mathcal{M}_m$, by (2.15)

$$\mathcal{M}_m \circ \#(E_\alpha^* \otimes E_\beta) = (\#(E_{\alpha'}^* \otimes E_{\beta'}) \circ \mathcal{M}_m)^\dagger = (\lambda_{\alpha_2}, \lambda_{\beta_2})_m (\#(E_{\alpha'}^* \otimes E_{\beta'}))^\dagger$$

form which (3.13) follows upon another application of (2.15). □

3.6 Theorem. *Let Φ be an Hermitian operator on $\mathfrak{H}$. Let $\{E_\alpha\}$ be the orthonormal basis of $\mathfrak{H}$ specified in (3.7), and let C_Φ be the characteristic matrix of Φ with respect to this basis. Then Φ is self-adjoint on $\mathcal{H}_m$ if and only if for all α, β,*

$$(c_\Phi)_{\alpha,\beta} = \frac{(\lambda_{\alpha_1}, \lambda_{\beta_1})_m}{(\lambda_{\alpha_2}, \lambda_{\beta_2})_m} (c_\Phi)_{\beta',\alpha'} \tag{3.14}$$

In particular, define the matrix $B_{\Phi,m}$ by

$$(b_{\Phi,m})_{\alpha,\beta} = (c_\Phi)_{\alpha,\beta} (\lambda_{\alpha_2}, \lambda_{\beta_2})_m \ , \tag{3.15}$$

and the anti-unitary self-adjoint operator U on $\mathbb{C}^{N^2}$ given by

$$(Uv)_\alpha = \overline{v_{\alpha'}} \ . \tag{3.16}$$

Then (3.17) is equivalent to

$$U B_{\Phi,m} = B_{\Phi,m} U \ . \tag{3.17}$$

Proof. Applying Lemma 3.4 together with Lemma 3.5 yields (3.14). Then (3.14) can be written as

$$(b_{\Phi,m})_{\alpha,\beta} = \overline{(b_{\Phi,m})}_{\alpha',\beta'} \ . \tag{3.18}$$

Then (3.17) follows from (3.16) and the definition of U. □

3.7 Remark. We may identify $\mathbb{C}^{N^2}$ equipped with its usual inner product and $\mathcal{M}_N(\mathbb{C})$ equipped with the Hilbert-Schmidt inner product in the usual way, identifying the vector v that has entries v_α with the matrix V that has entries V_{α_1,α_2}. Under this identification U is identified with V^*. That is, the anti-unitary map U may be identified with the map $V \mapsto V^*$.

3.1. QMS_m is always a pointed cone

3.8 Lemma. *An Hermitian operator $\mathscr{L}$ satisfies $\pm\mathscr{L} \in QMS$ if and only if for some H with $H = H^*$, $\mathscr{L}(A) = i[H, A]$.*

Proof. It is evident that if $\mathscr{L}(A) = i[H, A]$ with H self-adjoint, then both $\mathscr{L}$ and $-\mathscr{L}$ belong to QMS. For the converse, suppose that $\mathscr{L}$ and $-\mathscr{L}$ belong to QMS. Consider some unital orthonormal basis $\{F_\alpha\}$ of $\mathfrak{H}$. Let $C_{\mathscr{L}}$ be the characteristic matrix of $\mathscr{L}$ with respect to this basis. Since $\mathscr{L}$ and $-\mathscr{L}$ belong to QMS, the reduced characteristic matrix of $\mathscr{L}$ must be both positive semi-definite and negative semidefinite, and hence it is zero. Thus $(c_{\mathscr{L}})_{\alpha,\beta} = 0$ unless either $\alpha = (1,1)$ or $\beta = (1,1)$ or both. Since $\mathscr{L}$ is Hermitian $(c_{\mathscr{L}})_{(1,1),\beta} = \overline{(c_{\mathscr{L}})_{\beta,(1,1)}}$. Define

$$G := \frac{1}{2}(c_{\mathscr{L}})_{(1,1),(1,1)} + \sum_{\beta\neq(1,1)} (c_{\mathscr{L}})_{(1,1),\beta} F_\beta \ .$$

Then $\mathscr{L}(A) = \sum_{\alpha,\beta}(c_\Phi)_{\alpha,\beta} F_\alpha^* A F_\beta = G^*A + AG$. Write $G = K - iH$ with K and H self-adjoint. Since $\mathscr{L}(\mathbf{1}) = 0$, we have $G^* + G = 0$, that is, $K = 0$. Then $\mathscr{L}(A) = iHA - iAH = i[H, A]$. □

3.9 Theorem. *For any $m \in \mathcal{P}[0,1]$, the only Φ such that $\Phi \in QMS_m$ and $-\Phi \in QMS_m$ is $\Phi = 0$.*

Proof. Suppose that $\Phi \in QMS_m$ and $-\Phi \in QMS_m$. By Lemma 3.8, there is a self-adjoint $H \in \mathcal{M}_N(\mathbb{C})$ such that $\Phi(A) = i[H, A]$. Let $\{E_\alpha\}$ be the orthonormal basis of $\mathfrak{H}$ specified in (3.7), so that we may apply Theorem 3.6. We compute

$$\begin{aligned}(c_\Phi)_{\alpha,\beta} &= i\frac{1}{N^2}\sum_{i,j} \mathrm{Tr}\left[(E_\alpha^* E_{i,j} E_\beta)^*(HE_{i,j} - E_{i,j}H)\right] \\ &= i\frac{1}{N^2}\sum_{i,j} \mathrm{Tr}\left(\mathrm{Tr}[E_{i,j}E_\beta^* E_{j,i} E_\alpha H] - \mathrm{Tr}[R_{j,i}E_\alpha E_{i,j} H E_\beta^*]\right) \\ &= i\delta_{\beta_1,\beta_2}\langle E_\alpha^*, H\rangle_{\mathfrak{H}} - i\delta_{\alpha_1,\alpha_2}\langle E_\beta, H\rangle_{\mathfrak{H}} \ .\end{aligned}$$

In particular, $(c_\Phi)_{\alpha,\beta} = 0$ unless either $\alpha = \alpha'$ or $\beta = \beta'$ or both.

If $\alpha = \alpha'$ and $\beta = \beta'$, then

$$\langle E_\alpha^*, H\rangle_{\mathfrak{H}} = \frac{1}{N}\mathrm{Tr}[E_\alpha H] = \frac{1}{N}\mathrm{Tr}[HE_\alpha] \in \mathbb{R} \ ,$$

and likewise $\langle E_\beta, H\rangle_{\mathfrak{H}} \in \mathbb{R}$. But then $(c_\Phi)_{\alpha,\beta}$ is purely imaginary, and this contradicts (8.1) unless $(c_\Phi)_{\alpha,\beta} = 0$.

Next, suppose $\alpha = \alpha'$, but $\beta \neq \beta'$. Then

$$(c_\Phi)_{\alpha,\beta} = -i\langle E_\beta, H\rangle_{\mathfrak{H}} \quad \text{and} \quad (c_\Phi)_{\beta',\alpha} = i\langle E_\beta, H\rangle_{\mathfrak{H}} \ .$$

By (8.2) we then have

$$-(\lambda_{\alpha_2}, \lambda_{\beta_2})_m \langle E_\beta, H\rangle_{\mathfrak{H}} = (\lambda_{\alpha_2}, \lambda_{\beta_1})_m \langle E_\beta, H\rangle_{\mathfrak{H}} \ ,$$

which is impossible unless $\langle E_\beta, H\rangle_{\mathfrak{H}} = 0$. But since β is arbitrary apart from the condition that $\beta \neq \beta'$, this completes the proof that $H = 0$. □

3.2. The decomposition $\widehat{\mathfrak{H}} = \widehat{\mathfrak{H}}_{\mathcal{S}} \oplus \widehat{\mathfrak{H}}_{\mathcal{S}}^{\perp}$

Recall Definition 1.7 of $\widehat{\mathfrak{H}}_{\mathcal{S}}$ as the subspace of all operators Φ on $\widehat{\mathfrak{H}}$ of the form $\Phi(A) = XA + AY$ for some $X, Y \in \mathcal{M}_N(\mathbb{C})$.

3.10 Lemma. *An operator Φ on $\mathfrak{H}$ belongs to $\widehat{\mathfrak{H}}_{\mathcal{S}}$ if and only if for any unital orthonormal basis of $\mathfrak{H}$, the reduced characteristic matrix of Φ is zero; i.e., $R_\Phi = 0$.*

Proof. Let $\{F_\alpha\}$ be a unital orthonormal basis. Let $\{E_{i,j}\}$ be a matrix unit basis. Then for $\Phi(A) = XA + AY$ we compute

$$\begin{aligned}(c_\Phi)_{\alpha,\beta} &= \frac{1}{N^3}\sum_{i,j=1}^{N} \mathrm{Tr}[(F_\alpha^* E_{i,j} F_\beta)^*(XE_{i,j} + E_{i,j}Y)] \\ &= \frac{1}{N^3}(\mathrm{Tr}[F_\beta^*]\mathrm{Tr}[F_\alpha X] + \mathrm{Tr}[F_\alpha]\mathrm{Tr}[F_\beta^* Y]) \\ &= \frac{1}{N}(\delta_{\beta,(1,1)}\overline{\langle F_\alpha, X\rangle_{\mathfrak{H}}} + \delta_{\alpha,(1,1)}\langle F_\beta, Y\rangle_{\mathfrak{H}}) \end{aligned} \tag{3.19}$$

and this is zero unless either $\alpha = (1,1)$ or $\beta = (1,1)$ or both. Hence $R_\Phi = 0$.

On the other hand, if $R_\Phi = 0$, Φ has the form

$$\Phi(A) = (c_\Phi)_{(1,1),(1,1)} + \sum_{\alpha\neq(1,1)} (c_\Phi)_{\alpha,(1,1)} F_\alpha^* A + \sum_{\beta\neq(1,1)} (c_\Phi)_{(1,1),\beta} A F_\beta \ , \tag{3.20}$$

and hence if we define

$$X := \frac{1}{2}(c_\Phi)_{(1,1),(1,1)}\mathbf{1} + \sum_{\alpha\neq(1,1)} (c_\Phi)_{\alpha,(1,1)} F_\alpha^*$$

$$Y := \frac{1}{2}(c_\Phi)_{(1,1),(1,1)}\mathbf{1} + \sum_{\beta\neq(1,1)} (c_\Phi)_{(1,1),\beta} F_\beta$$

then Φ has the form $\Phi(A) = XA + AY$, and hence $\Phi \in \widehat{\mathfrak{H}}_{\mathcal{S}}$. □

3.11 Remark. By the computation in (3.19),

$$(c_\Phi)_{(1,1),(1,1)} = \frac{1}{N}\mathrm{Tr}[X^* + Y] = \overline{\langle E_{(1,1)}, X\rangle_{\mathfrak{H}}} + \langle E_{(1,1)}, Y\rangle_{\mathfrak{H}}$$

but for $\alpha \neq (1,1)$, both $\langle X, E_\alpha\rangle_{\mathfrak{H}}$ and $\langle Y, E_\alpha\rangle_{\mathfrak{H}}$ can be read off from C_Φ, so that if for some X', Y' we also have $\Phi(A) = X'A + AY'$, it follows that for some $\eta \in \mathbb{C}$, $X' = X + \eta\mathbf{1}$ and $Y' = Y - \overline{\eta}\mathbf{1}$.

3.12 Lemma. *Let Φ be CP with a minimal Kraus representation $\sum_{j=1}^M V_j^* A V_j$. Then the necessary and sufficient condition that $\Phi \in \widehat{\mathfrak{H}}_{\mathcal{S}}^{\perp}$ is that $\mathrm{Tr}[V_j] = 0$ for each j.*

Proof. Let $\{F_\alpha\}$ be any unit orthonormal basis. By Lemma 3.10 $\Phi \in \widehat{\mathfrak{H}}_{\mathcal{S}}^{\perp}$ if and only if the characteristic and reduced characteristic matrices of Φ, C_Φ and R_Φ, respectively, are such that the lower right $(N^2-1)\times(N^2-1)$ block of C_Φ is R_Φ and all other entries are zero. In other words, the first row and column of C_Φ are zero.

Writing $V_j = \sum_\alpha S_{j,\alpha} F_\alpha$, for some unit orthonormal basis $\{F_\alpha\}$,

$$\Phi(A) = \sum_{\alpha,\beta}\left(\sum_{j=1}^M (S_{\alpha,j}^* S_{j,\beta})\right) F_\alpha^* A F_\beta,$$

and hence

$$(c_\Phi)_{\alpha,\beta} = \sum_{j=1}^M (S_{\alpha,j}^* S_{j,\beta}) \ .$$

If for each j, $\mathrm{Tr}[V_j] = 0$, then $S_{(1,1),j} = 0$ for each j, and hence the first row and column of C_Φ are zero.

On the other hand, if the first row and column of C_Φ are zero, then

$$0 = (c_\Phi)_{(1,1),(1,1)} = \sum_{j=1}^M |S_{j,(1,1)}|^2 \ ,$$

and hence $S_{j,(1,1)} = 0$ for all j. This implies that $\mathrm{Tr}[V_j] = 0$. □

3.13 Lemma. *For all $s \in [0,1]$, the subspaces $\widehat{\mathfrak{H}}_{\mathcal{S}}$ and $\widehat{\mathfrak{H}}_{\mathcal{S}}^{\perp}$ are invariant under the operation of taking the adjoint on $\mathcal{H}_{\delta_s}$.*

Proof. Evidently it suffices to prove the invariance of $\widehat{\mathfrak{H}}_{\mathcal{S}}$. Let $\Phi(A) = XA + AY$. Then $\Phi^\dagger(A) = Y^*A + AX^*$ and so

$$\Phi^{*,\delta_s}(A) = (\Delta^{-s}Y^*)A + A(\Delta^{1-s}(G)X^*) \in \widehat{\mathfrak{H}}_{\mathcal{S}} \ . \quad \square \tag{3.21}$$

4. Self-adjointness for the KMS inner product

It is now very easy to determine the structure of $CP_{KMS} := CP_{\delta_{1/2}}$. In this case, (3.15) becomes

$$(b_{\Phi,m})_{\alpha,\beta} = \sqrt{\lambda_{\alpha_2}}(c_\Phi)_{\alpha,\beta}\sqrt{\lambda_{\beta_2}}\ . \tag{4.1}$$

Therefore, for Hermitian Φ, $B_{\Phi,KMS}$ is positive semi-definite if and only if C_Φ is positive semidefinite; i.e., if and only if Φ is CP.

4.1 Theorem. *Let $\mathfrak{K}$ be the real vector space consisting of all $V \in \mathcal{M}_N(\mathbb{C})$ such that $\Delta^{-1/2}V = V^*$. The extremal elements Φ of CP_{KMS} are precisely the elements of the form*

$$\Phi(A) = V^*AV\ , \qquad V \in \mathfrak{K}\ . \tag{4.2}$$

Every map in CP_{KMS} is a linear combination of at most N^2 such maps.

Proof. If Φ is extremal in the set of KMS self-adjoint CP maps, then necessarily C_Φ and $B_{\Phi,KMS}$ are rank one, because if $B_{\Phi,KMS}$ is not rank one, its spectral decomposition would allow it to be written as a sum of two positive matrices B_1 and B_2, neither a multiple of the other, and each commuting with U, the anti-unitary operator defined in Theorem 3.6. By Theorem 3.6, this would induce a decomposition of Φ into the sum of two KMS self-adjoint CP maps. It follows that Φ is extremal in the set of KMS self-adjoint CP maps if and only if $B = |u\rangle\langle u|$ where u is an eigenfunction of U; i.e., $Uu = \pm u$. Then

$$(c_\Phi)_{\alpha,\beta} = \frac{1}{\sqrt{\lambda_{\alpha_2}}}\overline{u_\alpha}u_\beta\frac{1}{\sqrt{\lambda_{\beta_2}}}$$

Thus if we define $V_u := \sum_\beta \frac{1}{\sqrt{\lambda_{\beta_2}}}u_\beta E_\beta$, then $\Phi(A) = V_u^*AV_u$.

Next, since

$$\Delta^{-1/2}E_\beta = \frac{\sqrt{\lambda_{\beta_2}}}{\sqrt{\lambda_{\beta_1}}}E_\beta\ ,$$

and hence, since $\overline{u_\beta} = \pm u_{\beta'}$,

$$\Delta^{-1/2}V_u = \sum_\beta \frac{1}{\sqrt{\lambda_{\beta_1}}}u_\beta E_\beta = \pm\sum_\beta \frac{1}{\sqrt{\lambda_{\beta_1}}}\overline{u_{\beta'}}E_\beta = \pm\sum_\beta \frac{1}{\sqrt{\lambda_{\beta_2}}}\overline{u_\beta}E_{\beta'} = \pm V_u^*\ .$$

Now suppose that V is such that $\Delta^{-1/2}V = \pm V^*$, and $\Phi(A) = V^*AV$. Then $\Phi^\dagger(A) = VAV^*$, and then by Lemma 3.4,

$$\Phi^{*,KMS}(A) = \sigma^{-1/2}(V(\sigma^{1/2}A\sigma^{1/2})V^*)\sigma^{-1/2} = (\Delta^{-1/2}V)^*A\Delta^{1/2}V = V^*AV = \Phi(A) \ .$$

Finally, observe that if $\Delta^{-1/2}V = -V^*$, then $\Delta^{-1/2}(iV) = (iV)^*$ and of course $V^*AV = (iV)^*A(iV)$, so we need only concern ourselves with V such that $\Delta^{-1/2}V = V^*$.

Now equip $\mathfrak{K}$ with the inner product

$$\langle V, W\rangle_{\mathfrak{K}} = \mathrm{Re}\ (\langle V, W\rangle_{\mathfrak{H}}) \ .$$

We will make use of the following orthonormal basis for $\mathfrak{K}$: Let $\{E_\alpha\}$ be a matrix unit basis associated to σ. First define

$$\omega_\alpha := \log\lambda_{\alpha_1} - \log\lambda_{\alpha_2} \ , \tag{4.3}$$

and note that $\Delta^{1/2}E_\alpha = e^{\omega_\alpha/2}E_\alpha$. For $\alpha = (\alpha_1, \alpha_2)$ such that $\alpha_1 < \alpha_2$, define

$$G_\alpha := \frac{1}{i\sqrt{2\cosh(\omega_\alpha/2)}}(e^{\omega_\alpha/4}E_\alpha - e^{-\omega_\alpha/4}E_\alpha^*) \ . \tag{4.4}$$

For $\alpha = (\alpha_1, \alpha_2)$ such that $\alpha_1 \geq \alpha_2$, define

$$G_\alpha := \frac{1}{\sqrt{2\cosh(\omega_\alpha/2)}}e^{\omega_\alpha/4}E_\alpha + e^{-\omega_\alpha/4}E_\alpha^* \ . \tag{4.5}$$

Then one readily checks that for all α,

$$\Delta^{-1/2}(G_\alpha) = G_\alpha^* \ , \tag{4.6}$$

and that $\{G_\alpha\}_{\alpha\in\mathcal{J}_N}$ is orthonormal in $\mathfrak{K}$.

We now show that $\{G_\alpha\}_{\alpha\in\mathcal{J}_N}$ is a basis for the real linear space in question. Suppose that $V \in \mathfrak{K}$. Let $\{E_\alpha\}$ be the modular basis out of which the orthonormal basis $\{G_\alpha\}$ was constructed. We then expand

$$V = \sum_\alpha a_\alpha e^{\omega_\alpha/4}E_\alpha \ .$$

We compute

$$\Delta^{-1/2}(V) = \sum_\alpha a_\alpha e^{-\omega_\alpha/4}E_\alpha \qquad \text{and} \qquad V^* = \sum_\alpha \overline{a_\alpha}e^{\omega_\alpha/4}E_\alpha^* = \sum_\alpha \overline{a_{\alpha'}}e^{\omega_{\alpha'}/4}E_\alpha \ .$$

It follows that since $\Delta^{-1/2}(V) = V^*$, then $a_\alpha e^{-\omega_\alpha/4} = \overline{a_{\alpha'}}e^{\omega_{\alpha'}/4} = \overline{a_{\alpha'}}e^{-\omega_\alpha/4}$, and hence $a_\alpha = \overline{a_{\alpha'}}$. Therefore, if $a_\alpha = x_\alpha + iy_\alpha$ is the decomposition of a_α into its real and imaginary parts,

$$a_\alpha e^{\omega_\alpha/4}E_\alpha + a_{\alpha'}e^{\omega_{\alpha'}/4}E_{\alpha'} = x_\alpha[e^{\omega_\alpha/4}E_\alpha + e^{-\omega_\alpha/4}E_\alpha^*] + iy_\alpha[e^{\omega_\alpha/4}E_\alpha - e^{-\omega_\alpha/4}E_\alpha^*]$$

Now consider any $\alpha = (\alpha_1, \alpha_2)$ with $\alpha_1 > \alpha_2$. Then we have

$$a_\alpha e^{\omega_\alpha/4} E_\alpha + a_{\alpha'} e^{\omega_{\alpha'}/4} E_{\alpha'} = x_\alpha G_\alpha + y_\alpha G_{\alpha'} \ ,$$

while if $\alpha_1 = \alpha_2$, $a_\alpha = a_{\alpha'} = x_\alpha$ and $a_\alpha e^{\omega_\alpha/4} E_\alpha + a_{\alpha'} e^{\omega_{\alpha'}/4} E_{\alpha'} = 2x_\alpha E_\alpha = x_\alpha G_\alpha$. Hence V is a real linear combination of the $\{G_\alpha\}$. □

4.2 Theorem. *Let Φ and Ψ be two CP maps that are KMS self-adjoint. Let $\Phi(A) = \sum_{j=1}^M V_j^* A V_j$ be a minimal Kraus representation of Φ with each $V_j \in \mathfrak{K}$. Then $\Phi - \Psi$ is CP if and only if there exists a real $M \times M$ matrix T such that $0 \le T \le \mathbf{1}$ and*

$$\Psi(A) = \sum_{i,j=1}^M T_{i,j} V_i^* A V_j \ . \tag{4.7}$$

Proof. Suppose that $\Phi - \Psi$ is CP. Then by Arveson's Theorem, there exists a uniquely determined T with $0 \le T \le \mathbf{1}$ such that (4.7) is valid. Since Ψ is KMS self-adjoint,

$$\Psi(A) = \sum_{i,j=1}^M \overline{T_{i,j}} \sigma^{-1/2} V_i \sigma^{1/2} A \sigma^{1/2} V_j^j \sigma^{-1/2} = \sum_{i,j=1}^M \overline{T_{i,j}} V_i^* A V_j \ .$$

By the uniqueness, T is real.

Conversely, suppose that Ψ has the form specified in (4.7) with $0 \le T \le \mathbf{1}$ and T is real. Then Φ is CP and KMS self-adjoint, and since $T \ge 0$, Ψ is CP, and since $T \le \mathbf{1}$, $\Phi \ge \Psi$. Finally, since T is real, Ψ is KMS self-adjoint. □

4.3 Theorem. *Let Φ be a unital CP map that is KMS self-adjoint and let $\Phi(A) = \sum_{j=1}^M V_j^* A V_j$ be a minimal Kraus representation of Φ with $V_j \in \mathfrak{K}$ for each j. Then Φ is an extreme point of the set of unital CP maps that are KMS self-adjoint if and only if*

$$\{V_i^* V_j + V_j^* V_i \ : \ 1 \le i \le j \le M\} \tag{4.8}$$

is linearly independent over the real numbers.

Proof. Suppose that the set in (4.8) is linearly independent over the real numbers. Suppose that Ψ is unital, CP and KMS self-adjoint, and that for some $0 < t < 1$, $\Phi - t\Psi$ is CP. We must show that $\Psi = \Phi$. By Lemma 4.2, there is a real $M \times M$ matrix T such that $0 \le T \le \mathbf{1}$ and

$$t\Psi(A) = \sum_{i,j=1}^M T_{i,j} V_i^* A V_j \ .$$

Then

$$t\mathbf{1} = t\Psi(\mathbf{1}) = \sum_{i,j=1}^{M} T_{i,j} V_i^* V_j \qquad \text{and} \qquad t\mathbf{1} = t\Phi(\mathbf{1}) = \sum_{i,j=1}^{M} t\delta_{i,j} V_i^* V_j \ .$$

Therefore

$$0 = \sum_{i,j=1}^{M} (t\delta_{i,j} - T_{i,j}) V_i^* V_j \ .$$

Then by the linear independence, $t\delta_{i,j} - T_{i,j} = 0$ for each i, j. Thus $t\Psi = t\Phi$, and Φ is extreme.

Now suppose that the set in (4.8) is not linearly independent over the reals. Then there is an $M \times M$ real symmetric matrix B such that $B_{i,j}$ are not all zero and $\sum_{i,j} B_{i,j} V_i^* V_j = 0$. Choose some $t > 0$ such that

$$0 \leq T := \mathbf{1} + tB \leq 2\mathbf{1} \ ,$$

and define Ψ by

$$\Psi(A) = \sum_{i,j=1}^{M} T_{i,j} V_i^* A V_j \ .$$

Then Ψ is CP, KMS self-adjoint, and

$$\Psi(\mathbf{1}) = \sum_{i,j=1}^{M} (\delta_{i,j} + tB_{i,j}) V_i^* A V_j = \sum_{i,j=1}^{M} \delta_{i,j} V_i^* \mathbf{1} V_j = \Phi(\mathbf{1}) = \mathbf{1} \ .$$

Thus Ψ is unital and since $\Psi \leq \frac{1}{2}\Phi$, Φ is not extreme. □

4.1. QMS_{KMS}

The problem of determining the structure of QMS generators that are self-adjoint on $\mathcal{H}_{KMS}$ has been studied in [6], but we give a simpler approach that goes further in one important aspect.

Let $\mathscr{L} \in QMS_{KMS}$ and write it in the form

$$\mathscr{L}(A) = (G^* A + AG) + \sum_{j=1}^{M} V_j^* A V_j \tag{4.9}$$

where $\{V_1, \ldots, V_M\}$ is linearly independent, which we may always do for any QMS generator. Replacing each V_j by $V_j - \mathrm{Tr}[V_j]\mathbf{1}$ and absorbing the difference into G, we may assume without loss of generality that for all j $\mathrm{Tr}[V_j] = 0$. By Lemma 3.12, Ψ, given by

$\Psi(A) = \sum_{j=1}^{M} V_j^* A V_j$ belongs to $\widehat{\mathfrak{H}}_{\mathcal{S}}^{\perp}$. Under these conditions on $\{V_1, \dots, V_M\}$, (4.9) is the orthogonal decomposition of $\mathscr{L}$ into its components in $\widehat{\mathfrak{H}}_{\mathcal{S}}$ and $\widehat{\mathfrak{H}}_{\mathcal{S}}^{\perp}$.

By Lemma 3.13, each component is individually self-adjoint. Let Φ denote the map $\Phi(A) = G^*A + AG$. Then $\Phi^\dagger(A) = GA + AG^*$ and hence

$$\Phi^{*,KMS}(A) = (\Delta^{-1/2}G)A + A(\Delta^{1/2}G^*)$$

Furthermore, adding a purely imaginary multiple of $\mathbf{1}$ to G has no effect on the operation $A \mapsto G^*A + AG$, and hence we may assume without loss of generality that $\mathrm{Tr}[G] \in \mathbb{R}$. Then $\mathrm{Tr}[\Delta^{-1/2}G] \in \mathbb{R}$, and by Remark 3.11, we must have $\Delta^{-1/2}G = G^*$.

Thus, a QMS generator $\mathscr{L}$ is self-adjoint on $\mathcal{H}_{KMS}$ if and only if it can be written in the form

$$\mathscr{L}(A) = G^*A + AG + \sum_{j=1}^{M} V_j^* A V_j \tag{4.10}$$

where $\mathrm{Tr}[G] \in \mathbb{R}$, $\{V_1, \dots, V_M\}$ is linearly independent, $\Delta^{-1/2}G = G^*$ and $\Delta^{-1/2}V_j = V_j^*$ as well as $\mathrm{Tr}[V_j] = 0$ for each j. As explained in the introduction, this much one finds in [6]. However, there is a compatibility question to be dealt with. Since $\mathscr{L}(\mathbf{1}) = 0$, we must have

$$0 = G^* + G + \sum_{j=1}^{M} V_j^* V_j \ . \tag{4.11}$$

That is, writing $G = H + iK$, H and K self-adjoint,

$$H = \frac{1}{2}\sum_{j=1}^{M} V_j^* V_j \ . \tag{4.12}$$

Now in general $\Delta^{-1/2}(H)$ is not even self-adjoint, so that $\Delta^{-1/2}(H) = H$ does not generally hold true.

This raises the following question: Given any CP map Ψ with a minimal Kraus representation $\Psi(A) = \sum_{j=1}^{M} V_j^* A V_j$ such that for each j $\Delta^{-1/2}V_j = V_j^*$ and $\mathrm{Tr}[V_j] = 0$, when does there exist a G such that

$$\mathscr{L}(A) := G^*A + AG + \Psi(A) \tag{4.13}$$

belongs to QMS_{KMS}? By what has been noted above, we may as well require $\mathrm{Tr}[G] \in \mathbb{R}$, and then we must have $\Delta^{-1/2}G = G^*$, and we must have $G = H + iK$, H and K self-adjoint, with H specified by (4.12). It turns out that there always exists a unique choice of K such that $\Delta^{-1/2}G = G^*$, and thus the answer to the question just raised is "always".

4.4 Theorem. *There is a one-to-one correspondence between elements $\mathscr{L}$ of QMS_{KMS} and CP maps $\Psi \in \widehat{\mathfrak{H}}_{\mathcal{S}}^{\perp}$ that are self-adjoint on $\mathcal{H}_{KMS}$. The correspondence identifies Ψ with $\mathscr{L}_\Psi$ where*

$$\mathscr{L}_\Psi(A) = G^*A + AG + \Psi(A) \tag{4.14}$$

where $G = H + iK$, H and K self-adjoint and given by

$$H := \tfrac{1}{2}\Psi(\mathbf{1}) \tag{4.15}$$

and

$$K := \frac{1}{i}\int_0^\infty e^{-t\sigma^{1/2}}(\sigma^{1/2}H - H\sigma^{1/2})e^{-t\sigma^{1/2}}\mathrm{d}t\ . \tag{4.16}$$

Furthermore, for all $\mathscr{L}_{\Psi_1}, \mathscr{L}_{\Psi_2} \in QMS_{KMS}$, $\mathscr{L}_{\Psi_1} - \mathscr{L}_{\Psi_2} \in QMS$ if and only if $\Psi_1 - \Psi_2 \in CP$; i.e., $\mathscr{L}_{\Psi_1} \geq \mathscr{L}_{\Psi_2}$ if and only if $\Psi_1 \geq \Psi_2$, and the extreme points of QMS_{KMS} are precisely the generators of the form

$$\mathscr{L}(A) := G^*A + AG + V^*AV$$

where $\Delta^{-1/2}V = V^*$ and where $G = H + iK$ is given by (4.15) and (4.16) for $\Psi(A) = V^*AV$.

Proof. Consider such a set $\{V_1, \dots V_M\}$ and define

$$\Psi(A) = \sum_{j=1}^{M} V_j^* A V_j\ . \tag{4.17}$$

Since $\mathrm{Tr}[V_j] = 0$ for each j, R_Ψ is positive semidefinite, and since $\Delta^{-1/2}V_j = V_j^*$ for each j, Ψ is self-adjoint on $\mathcal{H}_{KMS}$. Then for any choice of G, $\mathscr{L}(A) = G^*A + AG + \Psi(A)$ generates a CP semigroup, and it belongs to QMS if and only if $\mathscr{L}(\mathbf{1}) = 0$, and this is the case if and only if the self-adjoint part of $H := \frac{1}{2}(G + G^*)$ is given by (4.14). Finally, $\mathscr{L}$ will be self-adjoint on $\mathcal{H}_{KMS}$ if and only if $K := -i\frac{1}{2}(G - G^*)$ is chosen so that $\Delta^{-1/2}(G) = G^*$.

The equation $\Delta^{-1/2}(G) = G^*$ is equivalent to $(H + iK)\sigma^{1/2} = \sigma^{1/2}(H - iK)$, and rearranging terms we have

$$\sigma^{1/2}K + K\sigma^{1/2} = -i(\sigma^{1/2}H - H\sigma^{1/2})\ . \tag{4.18}$$

This is a Lyapunov equation, and for any X self-adjoint, the unique solution K of $\sigma^{1/2}K + K\sigma^{1/2} = X$ is given by

$$K := \int_0^\infty e^{-t\sigma^{1/2}} X e^{-t\sigma^{1/2}} \mathrm{d}t \ .$$

Indeed,

$$\sigma^{1/2} \left(\int_0^\infty e^{-t\sigma^{1/2}} X e^{-t\sigma^{1/2}} \mathrm{d}t \right) \sigma^{1/2} = - \int_0^\infty \frac{\mathrm{d}}{\mathrm{d}t} e^{-t\sigma^{1/2}} X e^{-t\sigma^{1/2}} \mathrm{d}t = X \ .$$

Thus we must take K to be given by (4.16). Note that $\mathrm{Tr}[K] = 0$ as an easy consequence of cyclicity of the trace, and hence $\mathrm{Tr}[G] \in \mathbb{R}$.

Now suppose $\mathscr{L}_{\Psi_1}, \mathscr{L}_{\Psi_2} \in QMS_{KMS}$. Then $\mathscr{L}_{\Psi_1} - \mathscr{L}_{\Psi_2} \in QMS$ if and only if its reduced density matrix is positive semidefinite. By Lemma 3.10 and Lemma 3.12, this is the case if and only if $\Psi_1 - \Psi_2$ is CP. The final assertion now follows from Theorem 4.1. □

5. Self-adjointness for the GNS inner product

The other case of main interest that is easily handled is the case of self-adjointness for the GNS inner product. While the KMS inner product corresponds to the measure $m = \delta_{1/2}$, the GNS inner product corresponds to the measure δ_0. It turns out that we may as well consider $m = \delta_s$, $s \neq \frac{1}{2}$; the set of CP maps that are self-adjoint on $\mathcal{H}_{\delta_s}$ does not depend on $s \neq \frac{1}{2}$. The structure of QMS_{GNS} was worked out by Alicki, and his methods adapt well to the study of $CP(\mathbf{1})_{GNS}$.

5.1 Theorem. *The extremal rays in the cone of CP maps that are self-adjoint on $\mathcal{H}_{\delta_s}$, $s \neq \frac{1}{2}$, are precisely the maps of the form*

$$\Phi(A) = e^{\omega/2} V^* A V + e^{-\omega/2} V A V^* \tag{5.1}$$

where $\Delta V = e^{\omega} V$, $\omega > 0$, or of the form

$$\Phi(A) = V A V \ , \tag{5.2}$$

$\Delta V = V = V^*$ In particular, every CP map that is self-adjoint on $\mathcal{H}_{\delta_s}$ is a positive linear combination of the operators specified in (5.1) and (5.2).

5.2 Remark. The restriction to $\omega > 0$ in (5.1) is not essential; it is to avoid double counting, since the eigenvalues e^{ω} of Δ with $\omega > 0$ and with $\omega < 0$ enter only in the precisely paired manner specified in (5.1). Also, note that replacing V by $e^{i\theta} V$, $\theta \in \mathbb{R}$, has no effect on the map in (5.2). There do exist V that are not self-adjoint such that $A \mapsto V^* A V$ is self-adjoint on $\mathcal{H}_{\delta_s}$ and extremal even in the wider class of all CP maps. However, the theorem asserts that in this case one may replace V by an appropriate complex multiple and then $V = V^*$.

Proof. Specializing to $m = \delta_s$, (3.14) becomes

$$(c_\Phi)_{\alpha,\beta} = \frac{\lambda_{\alpha_1}^s \lambda_{\beta_1}^{1-s}}{\lambda_{\alpha_2}^s \lambda_{\beta_2}^{1-s}} (c_\Phi)_{\beta',\alpha'} = e^{s\omega_\alpha + (1-s)\omega_\beta} (c_\Phi)_{\beta',\alpha'} \ . \tag{5.3}$$

As a consequence, $(c_\Phi)_{\beta',\alpha'} = e^{s\omega_{\beta'} + (1-s)\omega_{\alpha'}} (c_\Phi)_{\alpha,\beta} = e^{-s\omega_\beta - (1-s)\omega_\alpha} (c_\Phi)_{\alpha,\beta}$. Altogether,

$$e^{(1-2s)\omega_\alpha} (c_\Phi)_{\alpha,\beta} = (c_\Phi)_{\alpha,\beta} e^{(1-2s)\omega_\beta} \ . \tag{5.4}$$

That is, C_Φ commutes with the diagonal matrix Ω whose αth diagonal entry is $e^{(1-2s)\omega_\alpha}$. Of course this condition is vacuous for $s = \frac{1}{2}$, but otherwise it is a strong restriction on C_Φ. Let us order the entries in such a manner that all indices α for which e^{ω_α} has the same value are grouped together. Then C_Φ will have a block structure. In any case, as a consequence of (5.4), for $s \neq \frac{1}{2}$,

$$\omega_\alpha \neq \omega_\beta \ \Rightarrow \ (c_\Phi)_{\alpha,\beta} = 0 \ . \tag{5.5}$$

The blocks correspond to the distinct eigenvalues of the modular operator. Let μ be such an eigenvalue and let $\mathcal{J}_\mu = \{\alpha \ : \ e^{\omega_\alpha} = \mu \ \}$. Apart from $\mu = 1$, which is always an eigenvalue, the eigenvalues come in pairs. Let $\mu' := \frac{1}{\mu}$; then $\alpha \mapsto \alpha'$ is a one-to-one map from $\mathcal{J}_\mu$ onto $\mathcal{J}_{\mu'}$. For $\alpha, \beta \in \mathcal{J}_\mu$, (5.3) reduces to $(c_\Phi)_{\alpha,\beta} = \mu^{(1-2s)} (c_\Phi)_{\beta',\alpha'} = \mu^{(1-2s)} \overline{(c_\Phi)_{\alpha',\beta'}}$, or equivalently,

$$\mu^{-(1-2s)/2} (c_\Phi)_{\alpha,\beta} = \mu^{(1-2s)/2} \overline{(c_\Phi)_{\alpha',\beta'}} \ . \tag{5.6}$$

Hence, for $\mu \neq 1$, if $U_{\alpha,\beta}$, $\alpha, \beta \in \mathcal{J}_\mu$ is a unitary that diagonalizes the block corresponding to the eigenvalue μ, $\overline{U_{\alpha',\beta'}}$ is a unitary that diagonalizes the block corresponding to the eigenvalue $\frac{1}{\mu}$. For $\mu = 1$, (5.3) further reduces to $(c_\Phi)_{\alpha,\beta} = \overline{(c_\Phi)_{\alpha',\beta'}}$ which means that this block of C_Φ is diagonal in an orthonormal basis consisting of eigenvectors of this anti-unitary transformation. The eigenvectors v are such that

$$\left(\sum_{\alpha \in \mathcal{J}_1} v_\alpha E_\alpha \right)^* = \sum_{\alpha \in \mathcal{J}_1} \overline{v_\alpha} E'_\alpha = \pm \sum_{\alpha \in \mathcal{J}_1} v_\alpha E'_\alpha = \pm \sum_{\alpha \in \mathcal{J}_1} v_\alpha E_\alpha \ ,$$

commutes with the anti-unitary transformation $v_\alpha \mapsto \overline{v_{\alpha'}}$. Replacing v by $-v$ as needed, we can arrange that $\sum_{\alpha \in \mathcal{J}_1} v_\alpha E_\alpha$ is self-adjoint. Then the $\mu = 1$ block of C_Φ can be diagonalized by a unitary $U_{\gamma,\beta}$ such that for each $\gamma \in \mathcal{J}_1$, $\sum_{\beta \in \mathcal{J}_1} U_{\gamma,\beta} E_\beta$ is self-adjoint.

Now we piece together all the unitary blocks into an $N^2 \times N^2$ unitary that we still call U, being careful to use the "matched" unitaries in the adjoint blocks, as described above.

It follows that there is a unitary matrix U and non-negative numbers c_γ such that

$$c_{\alpha,\beta} = \sum_\gamma c_\gamma U^*_{\alpha,\gamma} U_{\gamma,\beta} = \sum_\gamma c_\gamma \overline{U_{\gamma,\alpha}} U_{\gamma,\beta}$$

and such that $U_{\gamma,\beta} = 0$ unless $e^{\omega_\gamma} = e^{\omega_\beta}$, and defining $V_\gamma := \sum_\beta U_{\gamma,\beta} E_\beta$ we have

$$\Delta V_\gamma = e^{\omega_\gamma} V_\gamma$$

for all γ and

$$\{V_\gamma \ : \ \gamma \in \mathcal{J}_N\} = \{V_\gamma^* \ : \ \gamma \in \mathcal{J}_N^*\}$$

is an orthonormal basis of $\mathfrak{H}$. When working with this basis, we redefine the map $\alpha \mapsto \alpha'$ by $V_{\alpha'} = V_\alpha^*$. This can only differ from the definition used with the matrix unit bases for indices in $\mathcal{J}_1$, and only if σ has at least two eigenvalues equal to one another, producing an "accidental" eigenvector of Δ with the eigenvalue 1.

Then $\Phi(A) = \sum_{\alpha,\beta} c_{\alpha,\beta} E_\alpha^* A E_\beta$ becomes $\Phi(A) := \sum_\gamma c_\gamma V_\gamma^* A V_\gamma$. Since $\Delta_\sigma(V_\gamma) = e^{\omega_\gamma} V_\gamma$ and $V_\alpha^* = V_{\alpha'}$

$$\begin{aligned}\Phi^{*,m_s}(A) &= \sum_\gamma \sigma^{-s} V_\gamma \sigma^s A \sigma^{1-s} V_\gamma^* \sigma^{-(1-s)} = \sum_\gamma c_\gamma e^{-s\omega_\gamma} e^{(s-1)\omega_\gamma} V_\gamma A V_\gamma^* \\ &= \sum_\gamma c_{\gamma'} e^{\omega_\gamma} V_\gamma^* A V_\gamma \ .\end{aligned}$$

By the uniqueness of the coefficients, $\Phi^{*,m_s} = \Phi$ if and only if for each γ

$$c_\gamma = c_{\gamma'} e^{\omega_\gamma} \ . \tag{5.7}$$

Defining $b_\gamma = e^{-\omega_\gamma/2} c_\gamma$, (5.7) is equivalent to $b_\gamma = b_{\gamma'}$. Let $\mathcal{S}$ denote the spectrum of Δ, which is of course determined by the spectrum of σ. We can finally write Φ in the form

$$\Phi(A) = \sum_{\gamma \in \mathcal{J}_1} c_\gamma V_\gamma A V_\gamma + \sum_{\mu \in \mathcal{S}, \mu > 1} \sum_{\gamma \in \mathcal{J}_\mu} b_\gamma \left(e^{\omega_\gamma/2} V_\gamma^* A V_\gamma + e^{-\omega_\gamma/2} V_\gamma A V_\gamma^* \right) \ . \tag{5.8}$$

It remains to show that the maps specified in (5.1) are extremal. Suppose first that $V = e^{i\theta} V^*$ for some real θ. Then $\omega = 0$, and (5.1) reduces to $\Phi(A) = V^* A V$ which is extremal in the larger cone of all CP maps, and thus extremal among those that are self-adjoint on $\mathcal{H}_{\delta_s}$. Replacing V by $e^{-i\theta/2} V$ we see that we may assume without loss of generality in this case that $V = V^*$.

Next, suppose that $V \neq e^{i\theta} V^*$ for any real θ, but $\omega = 0$. Write $V = X + iY$, X, Y self-adjoint. Then $\Delta X = X$ and $\Delta Y = Y$ and $X \neq Y$. We compute

$$\begin{aligned}V^* A V &= (X - iY) A (X + iY) = XAX + YAY + i(XAY - YAX) \\ V A V^* &= (X + iY) A (X - iY) = XAX + YAY - i(XAY - YAX) \ .\end{aligned}$$

Thus $\Phi(A) = XAX + YAY$. Then $A \mapsto XAX$ and $A \mapsto YAY$ are distinct CP maps that are self-adjoint on $\mathcal{H}_{\delta_s}$. Hence Φ is not extreme. In summary, when $\Delta V = V$, the

necessary and sufficient condition for Φ to be extremal is that $V^* = e^{i\theta}V$ for some real θ, in which case we may replace V by an equivalent self-adjoint operator.

Now suppose that $\Delta V = e^{\omega}V$ with $\omega \neq 0$. Then V and V^* are orthogonal. For convenience in what follows define $W_1 := e^{-(1-2s)\omega/4}V$ and $W_2 := e^{(1-2s)\omega/4}V^*$. Then, ignoring the trivial case $V = 0$,

$$\Phi(A) = W_1^* A W_1 + W_2^* A W_2$$

is a minimal Kraus representation of Φ. Consequently, if Ψ is any CP map such that $\Phi - \Psi$ is CP, then Ψ has the form

$$\Psi(A) = \sum_{i,j} T_{i,j} W_i^* A W_j$$

where T is a 2×2 matrix such that $0 \leq T \leq \mathbf{1}$. Then,

$$\Psi^{*,\delta_s}(A) = \sum_{i,j} \overline{T_{i,j}} (\Delta^{-s} W_i) A (\Delta^{1-s} W_j^*) = \sum_{i,j} \overline{T_{i,j}} e^{-s(3-2i)\omega} e^{(1-s)(3-2j)\omega} W_i A W_j^* \ .$$

Since $\overline{T_{i,j}} = T_{j,i}$, simple calculations yield

$$\Psi^{*,\delta_s}(A) = T_{1,1} W_2^* A W_2 + T_{2,2} W_1^* A W_1 + T_{2,1} e^{-\omega} W_1 A W_2^* + T_{1,2} e^{\omega} W_2 A W_1^* \ .$$

Then with $\Psi^{*,\delta_s} = \Psi$, by the uniqueness of the coefficients, $T_{1,2} = T_{2,1} = 0$ and $T_{1,1} = T_{2,2}$. This shows that T is a multiple of the identity, and hence that Ψ is a multiple of Φ. Hence Φ is extreme. □

The following notation will be useful going forward. For $\mu \in \mathcal{S}$, let d_μ be the dimension of the corresponding eigenspace of Δ. As a consequence of Theorem 5.1, every CP map Φ that is self-adjoint on $\mathcal{H}_{\delta_s}$ has a Kraus representation of the following form:

Let $\mathcal{S}' = \{\mu_1, \ldots, \mu_d\}$ be a subset of $\mathcal{S}$ such that $1 \leq \mu_1 \leq \mu_2 \cdots \leq \mu_d$. For each $1 \leq j \leq d$, let $\{V_1^{(j)}, \ldots, V_{M_j}^{(j)}\}$ be a linearly independent set of eigenvectors of Δ with eigenvalue μ_j. Evidently, $1 \leq M_j \leq d_j$. Suppose further that if $\mu_1 = 1$, then $\{V_1^{(1)}, \ldots, V_{M_1}^{(1)}\}$ is self-adjoint. Then, if $d_1 > 1$, the Kraus representation is

$$\Phi(A) = \sum_{j=1}^{d} \left(\sum_{k=1}^{M_j} (\mu_k^{1/2} V_k^{(j)*} A V_k^{(j)} + \mu_j^{-1/2} V_k^{(j)} A V_k^{(j)^*}) \right) \ , \tag{5.9}$$

while if $d_1 = 1$, it is

$$\Phi(A) = \sum_{k=1}^{M_1} V_k^{(1)} A V_k^{(1)} + \sum_{j=2}^{d} \left(\sum_{k=1}^{M_j} (\mu_j^{1/2} V_k^{(j)*} A V_k^{(j)} + \mu_j^{-1/2} V_k^{(j)} A V_k^{(j)^*}) \right) \ . \tag{5.10}$$

In either case, the minimality of the Kraus representation is a consequence of the linear independence required above. We call such a minimal Kraus representation of a CP map that is self-adjoint on $\mathcal{H}_{\delta_s}$, $s \neq \frac{1}{2}$ a *canonical minimal Kraus representation.*

5.3 Theorem. *Let Φ be a CP map that is self-adjoint on $\mathcal{H}_{\delta_s}$, $s \neq \frac{1}{2}$. Then if Ψ is another CP map that is self-adjoint on $\mathcal{H}_{\delta_s}$, $\Phi - \Psi$ is CP if and only if:*
(1) If Φ has a canonical minimal Kraus representation of the form (5.9), there are matrices $T^{(1)}, \dots, T^{(d)}$ where $T^{(j)}$ is an $M_j \times M_j$ matrix satisfying $0 \leq T^{(j)} \leq \mathbf{1}$ such that

$$\Psi(A) = \sum_{j=1}^{d} \left(\sum_{k,\ell=1}^{M_j} T^{(j)}_{k,\ell} \left(\mu_j^{1/2} V_k^{(j)*} A V_\ell^{(j)} + \mu_j^{-1/2} V_\ell^{(j)} A V_k^{(j)^*} \right) \right) , \tag{5.11}$$

(2) If Φ has a canonical minimal Kraus representation of the form (5.10), there are matrices $T^{(1)}, \dots, T^{(d)}$ where $T^{(j)}$ is an $M_j \times M_j$ matrix satisfying $0 \leq T^{(j)} \leq \mathbf{1}$, and with $T^{(1)}$ real, such that

$$\Psi(A) = \sum_{k,\ell=1}^{M_1} T^{(1)}_{k,\ell} V_k^{(1)} A V_\ell^{(1)} + \sum_{j=2}^{d} \left(\sum_{k,\ell=1}^{M_j} T^{(j)}_{k,\ell} \left(\mu_j^{1/2} V_k^{(j)*} A V_\ell^{(j)} + \mu_j^{-1/2} V_\ell^{(j)} A V_k^{(j)^*} \right) \right) . \tag{5.12}$$

Proof. Let us consider the case *(1)*. For each $j = 1, \dots, d$, apply the Gram-Schmidt algorithm to produce an invertible lower triangular $M_j \times M_j$ matrix $L^{(j)}$ and an orthonormal set $\{W_1^{(1)}, \dots, W_{M_j}^{(j)}\}$ such that

$$V_k^{(j)} = \sum_{\ell=1}^{M_j} L^{(j)}_{k,\ell} W_\ell^{(j)} \qquad \text{and hence} \qquad (V^{(j)})^*_k = \sum_{\ell=1}^{M_j} \overline{L^{(j)}_{k,\ell}} (W^{(j)})^*_\ell \, .$$

Evidently $\{W_1^{(1)}, \dots, W_{M_j}^{(j)}\}$ lies in the eigenspace of Δ corresponding to μ_j. Then

$$\Phi(A) = \sum_{j=1}^{d} \left(\sum_{k,\ell=1}^{M_j} \left(\mu_j^{1/2} [(L^{(j)})^* L^{(j)}]_{k,\ell} W_k^{(j)*} A W_\ell^{(j)} + \mu_j^{-1/2} \overline{[(L^{(j)})^* L^{(j)}]_{k,\ell}} W_k^{(j)} A W_\ell^{(j)^*} \right) \right) .$$

One can read off from this expression the characteristic matrix C_Φ with respect to the orthonormal basis obtained by extending, if necessary

$$\{ W_k^{(j)} \ : \ 1 \leq j \leq d \, , 1 \leq k \leq M_j \, \} \, .$$

Let C_Ψ denote the characteristic matrix of Ψ with respect to this same basis. Then $\Phi - \Psi$ is CP if and only if $C_\Phi - C_\Psi \geq 0$. Thus, $\Phi - \Psi$, which is certainly self-adjoint on $\mathcal{H}_{\delta_s}$, is CP if and only if there are matrices $\{R^{(1)}, \dots, R^{(d)}\}$ where for each j, $R^{(j)}$ is an $M_j \times M_j$ matrix with $0 \leq R^{(j)} \leq (L^{(j)})^* L^{(j)}$ such that

$$\Psi(A) = \sum_{j=1}^{d} \left(\sum_{k,\ell=1}^{M_j} \left(\mu_j^{1/2} R^{(j)}_{k,\ell} W^{(j)*}_k A W^{(j)}_\ell + \mu_j^{-1/2} \overline{R^{(j)}_{k,\ell}} W^{(j)}_k A W^{(j)^*}_\ell \right) \right) \ .$$

Now defining $T^{(j)} = ((L^{(j)})^{-1})^* R^{(j)} (L^{(j)})^{-1}$, we have the result in case *(1)* on account of the self-adjointness of each $T^{(j)}$.

The proof in case *(2)* is essentially the same, except for one point: Since $\{V_1^{(1)}, \dots, V_{M_1}^{(1)}\}$ is self-adjoint, for all i, j, $\mathrm{Tr}[(V_i^{(1)})^* V_j^{(1)}] = \mathrm{Tr}[V_i^{(1)} V_j^{(1)}] \in \mathbb{R}$.

Therefore, applying the Gram-Schmidt algorithm to $\{V_1^{(1)}, \dots, V_{M_1}^{(1)}\}$ yields a self-adjoint orthonormal basis $\{W_1^{(1)}, \dots, W_{M_1}^{(1)}\}$ and a *real* lower triangular matrix $L^{(1)}$ such that $V_k^{(1)} = \sum_{\ell=1}^{M_j} L^{(1)}_{k,\ell} W^{(1)}_\ell$. Also, since $\{W_1^{(1)}, \dots, W_{M_1}^{(1)}\}$ is a set of self-adjoint eigenvectors of Δ in the eigenspace with eigenvalue 1, $\sum_{j=1}^{M_1} R^{(1)}_{i,j} W^{(1)}_i A W^{(1)}_j$ is CP and self-adjoint on $\mathcal{H}_{\delta_s}$ if and only if $R^{(1)} \geq 0$ and $R^{(1)}$ is real. Hence the matrix $T^{(1)}$ is *real* in addition to satisfying $0 \leq T^{(1)} \leq \mathbf{1}$. □

5.4 Theorem. *Let $\Phi \in CP(\mathbf{1})_{\delta_s}$, the set of unital CP maps that are self-adjoint on $\mathcal{H}_{\delta_s}$. Let Φ have a canonical minimal Kraus representation specified in terms of*

$$\{ \ \{V_1^{(1)}, \dots, V_{M_1}^{(1)}\}, \dots, \{V_1^{(d)}, \dots, V_{M_d}^{(d)}\} \ \}$$

as in (5.9) *or* (5.10)*. Define*

$$X^{(j)}_{k,\ell} = \mu_j^{1/2} V^{(j)*}_k V^{(j)}_\ell + \mu_j^{-1/2} V^{(j)}_\ell V^{(j)^*}_k \ .$$

The necessary and sufficient condition for Φ to be extremal in $CP(\mathbf{1})_{\delta_s}$ is that for each $1 \leq j \leq d$,

$$\{ \ X^{(j)}_{k,\ell} \ : \ 1 \leq k, \ell \leq M_j \ , \ 1 \leq j \leq d \ \} \tag{5.13}$$

is linearly independent.

Proof. Suppose first that Φ has a canonical minimal Kraus representation of the type (5.9). Let Ψ be a unital CP map that is self-adjoint on $\mathcal{H}_{\delta_s}$, and suppose that for some $0 < t < 1$, $\Phi - t\Psi$ is CP. Then by Theorem 5.3, there are matrices $T^{(1)}, \dots, T^{(d)}$ where $T^{(j)}$ is an $M_j \times M_j$ matrix satisfying $0 \leq T^{(j)} \leq \mathbf{1}$ such that $t\Psi(A)$ is given by the right side of (5.11). Since Ψ and Φ are both unital, $t\Psi(\mathbf{1}) = t\Phi(1)$, and then

$$\sum_{j=1}^{d}\left(\sum_{k,\ell=1}^{M_j}(T_{k,\ell}^{(j)}-t\delta_{k,\ell})\left(\mu_j^{1/2}V_k^{(j)*}V_\ell^{(j)}+\mu_j^{-1/2}V_\ell^{(j)}V_k^{(j)^*}\right)\right)=0\ .$$

Then, if the set specified in (5.13) is linearly independent, for each j, $T^{(j)}=t\mathbf{1}$, and hence $t\Psi=t\Phi$ so that $\Psi=\Phi$. Hence Φ is extremal.

For the converse, suppose that the set specified in (5.13) is linearly dependent. Then there are matrices $\{B^{(1)},\dots,B^{(d)}\}$, not all zero, such that

$$\sum_{j=1}^{d}\left(\sum_{k,\ell=1}^{M_j}B_{k,\ell}^{(j)}\left(\mu_j^{1/2}V_k^{(j)*}V_\ell^{(j)}+\mu_j^{-1/2}V_\ell^{(j)}V_k^{(j)^*}\right)\right)=0\ . \tag{5.14}$$

The adjoint of the $N\times N$ matrix on the left in (5.14) equals the matrix obtained by replacing each $B^{(j)}$ by its adjoint. Thus, we may assume without loss of generality that each $B^{(j)}$ is self-adjoint.

Now replacing each $B^{(j)}$ with $tB^{(j)}$ for some common $t>0$, we may assume without loss of generality that $\|B^{(j)}\|\le 1$ for each j. Now define $T^{(j)}:=\frac{1}{2}(\mathbf{1}+B^{(j)})$. Then $0\le T^{(j)}\le\mathbf{1}$ for all j. Now, using these $T^{(j)}$, define Ψ by (5.11). Then by Theorem 5.3, Ψ is CP, self-adjoint on $\mathcal{H}_{\delta_s}$ and $\Phi-\Psi$ is CP. By (5.14) and the fact that Φ is unital, Ψ is unital. But since $B^{(j)}\neq 0$ for at least one j, Ψ is not a multiple of Φ. Hence Φ is not extremal.

The case in which Φ has a canonical minimal Kraus representation of the type (5.10) is quite similar. □

6. Evenly self-adjoint maps

We say a map Φ is *evenly self-adjoint* in case it is self-adjoint on $\mathcal{H}_m$ for all even m. Let CP_{even}, $CP_{even}(\mathbf{1})$ and QMS_{even} be the sets of evenly symmetric CP maps, unital CP maps and QMS generators respectively. We have seen that, for instance, $CP_{GNS}\subset CP_{even}\subset CP_{KMS}$, since when $\Phi\in CP_{GNS}$, Φ is self-adjoint on *every* $\mathcal{H}_m$ whether m is even or not, and since the measure m defining the KMS inner product is even. For the same reason we have $CP_{even}\subset CP_{BKM}$.

Using the next lemma, we will describe a natural way to construct elements of CP_{even}, $CP_{even}(\mathbf{1})$ and QMS_{even} that do not belong to CP_{GNS}, $CP_{GNS}(\mathbf{1})$ and QMS_{GNS} respectively:

6.1 Lemma. *Let $m\in\mathcal{P}[0,1]$ and suppose Φ is such that $[\mathcal{M}_m,\Phi]=0$. Then $\frac{1}{2}(\Phi+\Phi^\dagger)$ and $\frac{1}{2i}(\Phi-\Phi^\dagger)$ are self-adjoint on $\mathcal{H}_m$.*

Proof. By Lemma 3.4, Φ is self-adjoint on $\mathcal{H}_m$ if and only if $\mathcal{M}_m\circ\Phi=\Phi^\dagger\circ\mathcal{M}_m$. Since $\mathcal{M}_m^\dagger=\mathcal{M}_m$, $[\mathcal{M}_m,\Phi^\dagger]=0$. Then

$$\mathcal{M}_m\circ\tfrac{1}{2}(\Phi^\dagger+\Phi)=\tfrac{1}{2}(\Phi^\dagger+\Phi)\circ\mathcal{M}_m=\tfrac{1}{2}(\Phi^\dagger+\Phi)^\dagger\circ\mathcal{M}_m\ .$$

The proof for $\frac{1}{2i}(\Phi - \Phi^\dagger)$ is the same. □

For $1 \leq i, j \leq N$, let $E_{i,j} := \sqrt{N}|u_i\rangle\langle u_j|$ where $\{u_1, \dots, u_N\}$ is an orthonormal basis of $\mathbb{C}^N$ consisting of eigenvectors of σ; $\sigma u_j = \lambda_j u_j$. Recall that the $E_{i,j}$ are an orthonormal basis of $\mathfrak{H}$ consisting of eigenvectors of $\mathcal{M}_m$ with $\mathcal{M}_m E_{i,j} = (\lambda_i, \lambda_j)_m E_{i,j}$. If m is not even, it can easily be that each eigenspace of $\mathcal{M}_m$ is one dimensional, and then Φ commutes with $\mathcal{M}_m$ if and only if it is a function of $\mathcal{M}_m$ itself.

However, when m is even, $(\lambda_i, \lambda_j)_m = (\lambda_j, \lambda_i)_m$ for all i, j, and hence if $i < j$, $E_{i,j}$ and $E_{j,i}$ belong to the same eigenspace. For $i < j$, consider the map Φ defined by $\Phi(A) = E_{i,j}AE_{i,j}$. Note that $\Phi^\dagger(A) = E_{j,i}AE_{j,i}$. A simple calculation shows that $\Phi \circ \mathcal{M}_m = (\lambda_i, \lambda_j)_m \Phi$ and $\mathcal{M}_m \circ \Phi = (\lambda_j, \lambda_i)_m \Phi$. Hence, whenever m is even, $[\Phi, \mathcal{M}_m] = 0$. For $i \neq j$ define the maps $\Psi_{i,j}$ by

$$\Psi_{i,j}(A) := \begin{cases} \frac{1}{2}(E_{i,j}AE_{i,j} + E_{j,i}AE_{j,i}) & i < j \\ \frac{1}{2i}(E_{i,j}AE_{i,j} - E_{j,i}AE_{j,i}) & i > j \ . \end{cases} \tag{6.1}$$

Lemma 6.1 says that these maps are evenly self-adjoint.

Therefore, let Φ_0 be a CP map that is self-adjoint on $\mathcal{H}_m$ for all $m \in \mathcal{P}[0,1]$, and let T be a real $N \times N$ matrix that is zero on the diagonal. Then

$$\Phi = \Phi_0 + \sum_{i \neq j} T_{i,j} \Psi_{i,j} \tag{6.2}$$

is evenly self-adjoint, and is CP if and only if $C_{\Phi_0 + \sum_{i \neq j} T_{i,j}\Psi_{i,j}} \geq 0$. Notice also that $\Psi_{i,j}(\mathbf{1}) = 0$ for all $i \neq j$, so that, if Φ_0 is unital, then so is the operator Φ in (6.2). Likewise, if $\mathscr{L}_0$ is a QMS generator that is self-adjoint on $\mathcal{H}_m$ for all $m \in \mathcal{P}[0,1]$, then

$$\mathscr{L} = \mathscr{L}_0 + \sum_{i \neq j} T_{i,j} \Psi_{i,j} \tag{6.3}$$

is evenly self-adjoint, and is a QMS generator if and only if $R_{\mathscr{L}_0 + \sum_{i \neq j} T_{i,j}\Psi_{i,j}} \geq 0$ where the reduced density matrix is computed with respect to any unital basis.

As we explain next, under a non-degeneracy condition on the spectrum of the modular operator, this construction not only gives us a class of examples, but a complete parameterization of the set of all evenly self-adjoint CP maps and QMS generators.

Suppose the eigenvalues $\{\lambda_1, \dots, \lambda_N\}$ of σ are such that the $N^2 - N$ numbers $\frac{\lambda_i}{\lambda_j}$, $i \neq j$ are all distinct, which of course implies that the N eigenvalues of σ are all distinct. In this case we say that the modular operator has *minimally degenerate spectrum* – the eigenvalue 1 has multiplicity N and all other eigenvalues are simple.

6.2 Theorem. *Suppose σ is such that Δ has minimally degenerate spectrum. Let Φ be an evenly self-adjoint CP map. Then there exists a GNS self-adjoint CP map Φ_0 and a real*

$N \times N$ matrix T that is zero on the diagonal such that Φ is given by (6.2). If we also assume $\Phi \in CP(\mathbf{1})$, then $\Phi_0 \in CP(\mathbf{1})$.

Furthermore, the extreme points of the set CP_{even} of evenly self-adjoint CP maps are of the form either

$$\Phi(A) = VAV \tag{6.4}$$

where $\Delta(V) = V$ and $V^* = V$, in which case Φ is GNS self-adjoint, or, for some α such that $\alpha_1 < \alpha_2$,

$$\Phi(A) = a\left(\lambda_{\alpha_1} E_{\alpha'} A E_\alpha + \lambda_{\alpha_2} E_\alpha A E_{\alpha'} + \sqrt{\lambda_{\alpha_1}\lambda_{\alpha_2}}(e^{i\theta} E_{\alpha'} A E_{\alpha'} + e^{-i\theta} E_\alpha A E_\alpha)\right) \tag{6.5}$$

where $a > 0$ and $\theta \in [0, 2\pi)$, in which case Φ is not GNS self-adjoint.

6.3 Theorem. *Suppose σ is such that Δ has minimally degenerate spectrum. Let $\mathscr{L}$ be an evenly self-adjoint QMS generator. Then there exists a GNS self-adjoint CP map $\mathscr{L}_0$ and a real $N \times N$ matrix T that is zero on the diagonal such that $\mathscr{L}$ is given by (6.3). Furthermore, the extreme points of the set QMS_{even} of evenly self-adjoint QMS generators are of the form either*

$$\mathscr{L}(A) = VAV - \tfrac{1}{2}(V^2 A + AV^2) \tag{6.6}$$

where $\Delta(V) = V$ and $V^* = V$, in which case $\mathscr{L}$ is GNS self-adjoint, or, for some α such that $\alpha_1 < \alpha_2$,

$$\mathscr{L}(A) = a\left(\lambda_{\alpha_1} E_{\alpha'} A E_\alpha + \lambda_{\alpha_2} E_\alpha A E_{\alpha'} + \sqrt{\lambda_{\alpha_1}\lambda_{\alpha_2}}(e^{i\theta} E_{\alpha'} A E_{\alpha'} + e^{-i\theta} E_\alpha A E_\alpha)\right) \tag{6.7}$$

$$- \tfrac{a\sqrt{N}}{2}\left((\lambda_{\alpha_1} E_{\alpha_2,\alpha_2} + \lambda_{\alpha_2} E_{\alpha_1,\alpha_1})A + A(\lambda_{\alpha_1} E_{\alpha_2,\alpha_2} + \lambda_{\alpha_2} E_{\alpha_1,\alpha_1})\right), \tag{6.8}$$

where $a > 0$ and $\theta \in [0, 2\pi)$, in which case $\mathscr{L}$ is not GNS self-adjoint.

The proofs of these theorems are very similar. We first record some useful lemmas.

6.4 Lemma. *Let $a, b, c, d > 0$ with $a \le b$ and $c \le d$. Then*

$$\frac{(a,b)_m}{(c,d)_m} \tag{6.9}$$

is independent of the even measure m if and only if $\frac{a}{c} = \frac{b}{d}$.

Proof. Suppose $\frac{a}{c} = \frac{b}{d} = K$. Then $a = Kc$ and $b = Kd$ so that for any m,

$$\int_0^1 a^s b^{1-s} \mathrm{d}m = \int_0^1 (Kc)^s (Kd)^{1-s} \mathrm{d}m = K \int_0^1 c^s d^{1-s} \mathrm{d}m \ ,$$

and the ratio in (6.9) is independent of m, even or not.

For the converse, suppose that the ratio in (6.9) is K for all even m. Then taking $m = \delta_{1/2}$ and $m = \frac{1}{2}(\delta_0 + \delta_1)$, giving the geometric and arithmetic means respectively, we have

$$a + b = K(c + d) \quad \text{and} \quad \sqrt{ab} = K\sqrt{cd} \ ,$$

from which we deduce

$$(\sqrt{a} + \sqrt{b})^2 = K(\sqrt{c} + \sqrt{d})^2 \quad \text{and} \quad (\sqrt{a} - \sqrt{b})^2 = K(\sqrt{c} - \sqrt{d})^2$$

Since $a \leq b$ and $c \leq d$,

$$\sqrt{a} = \frac{\sqrt{a} + \sqrt{b}}{2} + \frac{\sqrt{a} - \sqrt{b}}{2} = \sqrt{K}\frac{\sqrt{c} + \sqrt{d}}{2} + \sqrt{K}\frac{\sqrt{c} - \sqrt{d}}{2} = \sqrt{K}\sqrt{c} \ ,$$

and likewise, $\sqrt{b} = \sqrt{K}\sqrt{d}$. This implies that $\frac{a}{c} = \frac{b}{d} = K$. □

6.5 Lemma. *Let Φ be an evenly symmetric map. Suppose $1 \leq i, j, k, \ell \leq N$ are such that there exist even m_1 and m_2 for which*

$$\frac{(\lambda_i, \lambda_k)_{m_1}}{(\lambda_j, \lambda_\ell)_{m_1}} \neq \frac{(\lambda_i, \lambda_k)_{m_2}}{(\lambda_j, \lambda_\ell)_{m_2}} \tag{6.10}$$

Let C_Φ be the characteristic matrix of $\mathscr{L}$ computed with respect to $\{E_{i,j}\}$. Then $(c_\Phi)_{(i,j),(k,\ell)} = 0$.

Proof. By Theorem 3.6, for Φ to be self-adjoint on $\mathcal{H}_{m_1}$,

$$(c_\Phi)_{(i,j),(k,\ell)} = \frac{(\lambda_i, \lambda_k)_{m_1}}{(\lambda_j, \lambda_\ell)_{m_1}} (c_\Phi)_{(\ell,k),(j,i)} \ ,$$

while for Φ to be self-adjoint on $\mathcal{H}_{m_2}$, the same relation must hold with m_1 replaced by m_2. By (6.10), this means that $(c_\Phi)_{(i,j),(k,\ell)} = 0$. □

Proof of Theorem 6.2. Returning to the notation $\alpha = (\alpha_1, \alpha_2)$ and $\alpha' = (\alpha_2, \alpha_1)$, by Lemma 6.5, $(c_\Phi)_{\alpha,\beta} = 0$ unless $\frac{(\lambda_{\alpha_1}, \lambda_{\beta_1})_m}{(\lambda_{\alpha_2}, \lambda_{\beta_2})_m}$ is independent of m even. By Lemma 6.4, this means that either

$$\frac{\lambda_{\alpha_1}}{\lambda_{\alpha_2}} = \frac{\lambda_{\beta_1}}{\lambda_{\beta_2}} \quad \text{or} \quad \frac{\lambda_{\alpha_1}}{\lambda_{\beta_2}} = \frac{\lambda_{\beta_1}}{\lambda_{\alpha_2}} \ .$$

Since the spectrum of Δ is minimally degenerate, the first of these conditions is satisfied if and only if either ($\alpha = \beta$) or ($\alpha = \alpha'$ and $\beta = \beta'$). The second of these conditions is satisfied if and only if $\alpha = \beta$ or $\alpha = \beta'$. Thus, when Δ has minimally degenerate spectrum and Φ is evenly self-adjoint, then $(c_\Phi)_{\alpha,\beta} = 0$ unless one of the following is satisfied:

(1) $\alpha = \alpha'$ and $\beta = \beta'$
(2) $\alpha = \beta$
(3) $\alpha = \beta'$

If we order the indices so that $(1,1), \dots, (N,N)$ come first, followed by consecutive pairs (i,j) and (j,i) with $i < j$, C_Φ will have an $N \times N$ block in the upper left, and then a string of $\binom{N}{2}$ 2×2 blocks down the diagonal, with all other entries being zero. Consider one of these 2×2 blocks. The diagonal entries are $(c_\Phi)_{\alpha,\alpha}$ and $(c_\Phi)_{\alpha',\alpha'}$ for some α with $\alpha_1 < \alpha_2$. Again by Theorem 3.6, these are related by

$$(c_\Phi)_{\alpha,\alpha} = \frac{\lambda_{\alpha_1}}{\lambda_{\alpha_2}} (c_\Phi)_{\alpha',\alpha'}$$

Hence if we order the indices so that α comes before α', the 2×2 block has the form

$$a \begin{bmatrix} \lambda_{\alpha_1} & \zeta \\ \overline{\zeta} & \lambda_{\alpha_2} \end{bmatrix}$$

for some $a \geq 0$. Then if $a \neq 0$, we must have $|\zeta|^2 \leq \lambda_{\alpha_1}\lambda_{\alpha_2}$ if Φ is completely positive. If we write $\zeta = x + iy$, $x, y \in \mathbb{R}$, then

$$a \begin{bmatrix} \lambda_{\alpha_1} & \zeta \\ \overline{\zeta} & \lambda_{\alpha_2} \end{bmatrix} = a \begin{bmatrix} \lambda_{\alpha_1} & 0 \\ 0 & \lambda_{\alpha_2} \end{bmatrix} + x\Psi_{\alpha_1,\alpha_2} + y\Psi_{\alpha_2,\alpha_1} \ . \tag{6.11}$$

Applying this to all such blocks we see that Φ has the form

$$\Phi = \Phi_0 + \sum_{i \neq j} T_{i,j} \Psi_{i,j} \tag{6.12}$$

where C_{Φ_0} is the matrix obtained by setting all off diagonal elements of C_Φ outside the upper left $N \times N$ block equal to zero. Since C_Φ is positive semidefinite, so is C_{Φ_0}. It follows that Φ_0 is CP and GNS symmetric. Also note that $\Phi(\mathbf{1}) = \mathbf{1}$ is equivalent to $\Phi_0(\mathbf{1}) = \mathbf{1}$, since the maps $\Psi_{i,j}$ annihilate $\mathbf{1}$.

Maps of the form (6.4) are readily seen to be extreme points of CP_{even}, just as in the proof of Theorem 5.1. Other extrema Φ are obtained by letting the only non-zero entries in C_Φ be those of a 2×2 block like (6.11) with $|\zeta|$ chosen as to give equality in the condition $|\zeta|^2 \leq \lambda_{\alpha_1}\lambda_{\alpha_2}$. These extreme points are those of the form (6.5). In particular

note that maps of the form (5.1), which were extreme in CP_{GNS}, are not extreme in CP_{even}, since they can be obtained as convex combinations of two maps in the form (6.5) using opposite values of θ. □

Proof of Theorem 6.3. Just as in the proof of Theorem 6.2 above, we conclude that $C_{\mathscr{L}}$ for an evenly self-adjoint QMS generator $\mathscr{L}$ has the block structure of an upper-left $N \times N$ block followed by $\binom{N}{2}$ 2×2 blocks down the diagonal in the form (6.11), which justifies the formula

$$\mathscr{L} = \mathscr{L}_0 + \sum_{i \neq j} T_{i,j} \Psi_{i,j} \tag{6.13}$$

with $\mathscr{L}_0$ being GNS self-adjoint. It remain to prove that $\mathscr{L}_0$ is a QMS generator.

According to Lemma 2.8, the reduced characteristic matrix $R_{\mathscr{L}}$ of $\mathscr{L}$ computed in some unital orthonormal basis must be positive semidefinite. Moreover, as a consequence of Lemma 2.2 and as described in Remark 2.6, $R_{\mathscr{L}}$ can be obtained as the lower-right (N^2-1)-dimensional block of the matrix $\widetilde{C}_{\mathscr{L}} = UC_{\mathscr{L}}U^*$, where U is an unitary matrix containing a nonzero upper-left $N \times N$ block and the identity for its lower-right $(N^2-N) \times (N^2-N)$ block. In particular $R_{\mathscr{L}}$ has a block structure with an upper-left $(N-1) \times (N-1)$ block and the same $\binom{N}{2}$ 2×2 blocks down the diagonal as $C_{\mathscr{L}}$, and by assumption each of these blocks is positive semidefinite, which implies the same condition $|\zeta|^2 \leq \lambda_{\alpha_1}\lambda_{\alpha_2}$ described in the proof of the previous theorem. Meanwhile, $R_{\mathscr{L}_0}$ also has a block structure with the same upper-left $(N-1) \times (N-1)$ block as $R_{\mathscr{L}}$ (because the upper-left $N \times N$ blocks for $C_{\mathscr{L}}$ and $C_{\mathscr{L}_0}$ are the same), and with a diagonal lower-right $(N^2-N) \times (N^2-N)$ block. Hence $R_{\mathscr{L}_0}$ is positive semidefinite, implying that $\mathscr{L}_0$ is a QMS generator.

The description of the extreme points of QMS_{even} follows the same reasoning as in the proof of Theorem 6.2 above. □

7. From KMS self-adjointness to BKM self-adjointness

Recall that $\mathcal{M}_{BKM}$ denotes the operator on $\mathfrak{H}$ given by

$$\mathcal{M}_{BKM}(A) = \int_0^1 \sigma^s A \sigma^{1-s} \mathrm{d}s \ . \tag{7.1}$$

Then

$$\mathcal{M}_{BKM}^{-1}(A) = \int_0^\infty \frac{1}{t+\sigma} A \frac{1}{t+\sigma} \mathrm{d}t \ , \tag{7.2}$$

so that $\mathcal{M}_{BKM}^{-1}$ is CP. Now define the unital CP map

$$\Psi(A) = \int_0^\infty \frac{\sqrt{\sigma}}{t+\sigma} A \frac{\sqrt{\sigma}}{t+\sigma} \mathrm{d}t \ . \tag{7.3}$$

7.1 Theorem. *The map $\Phi \mapsto \Psi \circ \Phi$ is a one-to-one map from the set of KMS self-adjoint CP maps into the set of BKM self-adjoint CP maps, taking unital maps to unital maps.*

Proof. Let Φ be KMS self-adjoint. Then

$$\begin{aligned}
\langle B, \Psi(\Phi(A))\rangle_{BKM} &= \mathrm{Tr}[B^* \mathcal{M}_{BKM}(\Psi(\Phi(A)))] \ = \mathrm{Tr}[B^* \sqrt{\sigma}\Phi(A)\sqrt{\sigma}] \\
&= \langle B, \Phi(A)\rangle_{KMS} = \langle \Phi(B), A\rangle_{KMS} \\
&= \mathrm{Tr}[\sqrt{\sigma}(\Phi(B))^*\sqrt{\sigma}A] = \mathrm{Tr}[\mathcal{M}_{BMK}^{-1}(\sqrt{\sigma}(\Phi(B))^*\sqrt{\sigma}), \mathcal{M}_{BKM}(A)] \\
&= \langle \Psi(\Phi(B)), A\rangle_{BKM} \ .
\end{aligned}$$

The rest follows from the fact that Ψ is invertible, CP, and unital. □

Evidently, a similar construction is possible for any m such that $\mathcal{M}_m^{-1}$ is CP. This is not the case for every even m, but there are examples other than BKM and KMS:

7.2 Theorem. *For $s \in [0,1]$ define $m_s := \frac{1}{2}(\delta_s + \delta_{1-s})$. Then for each $s \in [0,1]$, the operator $\mathcal{M}_{m_s}^{-1}$ is completely positive for all $\sigma \in \mathfrak{S}_+$.*

Proof. By Lemma 3.2, for any m, for the standard matrix unit basis $\{E_\alpha\}$,

$$(c_{\mathcal{M}_m^{-1}})_{\alpha,\beta} = (\alpha_1, \beta_1)_m^{-1} \delta_{\alpha_1,\alpha_2}\delta_{\beta_1,\beta_2} \ .$$

If we order the indices as usual so that $(1,1), \dots, (N,N)$ come first, $C_{\mathcal{M}_m}$ has the $N \times N$ matrix $\Lambda^{(m)}$ defined by

$$\Lambda_{i,j}^{(m)} := \frac{1}{(\lambda_i, \lambda_j)_m} \tag{7.4}$$

in its upper left block, and is zero elsewhere. By Lemma 2.4 $\mathcal{M}_m^{-1}$ is CP if and only if $\Lambda^{(m)}$ is positive semi-definite. Specializing to the case $m = m_s$ for some s,

$$\Lambda_{i,j}^{(m_s)} = \lambda_i^{-s}\lambda_j^{-s}\frac{2}{\lambda_i^{1-2s} + \lambda_j^{1-2s}} \ .$$

Define $\kappa_j = \lambda_j^{1-2s}$. Then

$$\frac{1}{\lambda_i^{1-2s} + \lambda_j^{1-2s}} = \int_0^1 t^{\kappa_i + \kappa_j - 1} \mathrm{d}t \ ,$$

and hence for any $(z_1, \dots, z_n) \in \mathbb{C}^n$,

$$\sum_{i,j=1}^{n} z_i^* \Lambda_{i,j}^{(m_s)} z_j = 2 \int_0^1 \left| \sum_{i=1}^{n} \lambda_i^{-s} t^{\kappa_i - \frac{1}{2}} z_i \right|^2 \mathrm{d}t \geq 0 \ ,$$

proving that $\Lambda^{(m_s)}$ is positive semidefinite. □

8. QMS_m for $N = 2$, m even

The following lemma will facilitate the computations in this section:

8.1 Lemma. *Let Φ be self-adjoint on $\mathcal{H}_m$. Then, with respect to any matrix unit orthonormal basis of $\mathfrak{H}$, the characteristic matrix C_Φ of Φ satisfies*

$$\text{For } \alpha = \alpha', \beta = \beta' \ , \quad (c_\Phi)_{\alpha,\beta} = (c_\Phi)_{\beta,\alpha} \ , \tag{8.1}$$

$$\text{For } \alpha = \alpha', \beta \neq \beta' \ , \quad (c_\Phi)_{\alpha,\beta}(\lambda_{\alpha_2}, \lambda_{\beta_2})_m = (c_\Phi)_{\beta',\alpha}(\lambda_{\alpha_2}, \lambda_{\beta_1})_m \ , \tag{8.2}$$

$$\text{For } \alpha \neq \alpha' \ , \ \alpha = \beta' \ , \quad (c_\Phi)_{\alpha,\beta}(\lambda_{\alpha_2}, \lambda_{\alpha_1})_m = (c_\Phi)_{\alpha,\beta}(\lambda_{\alpha_1}, \lambda_{\alpha_2})_m \ , \tag{8.3}$$

$$\text{For } \alpha \neq \alpha' \ , \ \alpha = \beta \ , \quad (c_\Phi)_{\alpha,\beta}\lambda_{\alpha_2} = (c_\Phi)_{\alpha,\beta}\lambda_{\alpha_1} \ , \tag{8.4}$$

Proof. This is an immediate consequence of Theorem 3.6. □

In this section we determine the structure of QMS_m for even m when $N = 2$. First consider any Hermitian $\mathscr{L}$ on $\mathcal{M}_2(\mathbb{C})$ such that $\mathscr{L}(\mathbf{1}) = 0$. Then the fact that $C_\mathscr{L}$ is self-adjoint, together with Lemma 2.9 constrain $C_\mathscr{L}$ to have the form

$$C_\mathscr{L} = \begin{bmatrix} -a & \zeta_1 & z & \zeta_2 \\ \overline{\zeta_1} & -b & \zeta_4 & -\overline{z} \\ \overline{z} & \overline{\zeta_4} & b & \zeta_3 \\ \overline{\zeta_2} & -z & \overline{\zeta_3} & a \end{bmatrix} \ , \tag{8.5}$$

where a, b are real and z is complex and the relations among entries involving them are determined by Lemma 2.9 and self-adjointness, and where $\zeta_1, \dots, \zeta_4$ are complex, and the relations among entries involving them are constrained only by self-adjointness.

We next apply Lemma 8.1. By (8.1), $\zeta_1 = \zeta_1^* =: -x$, and hence the upper-left block is real and symmetric for all choices of m. By (8.3), since $(\lambda_1, \lambda_2)_m = (\lambda_2, \lambda_1)_m$ there is no restriction on ζ_3.

Next we apply (8.2). Taking $\alpha = (1,1)$ and $\beta = (1,2)$, and then $\alpha = (2,2)$ and $\beta = (2,1)$, we see that

$$z = \frac{\lambda_1}{(\lambda_1, \lambda_2)_m} \overline{\zeta_2} \quad \text{and} \quad -z = \frac{\lambda_2}{(\lambda_2, \lambda_1)_m} \zeta_4 \ .$$

Next we apply (8.4). Taking $\alpha = (1,2)$ and $\beta = (1,2)$

$$b = \frac{\lambda_1}{\lambda_2} a \ .$$

We conclude that if we set $\mu_j := (\lambda_1, \lambda_2)_m / \lambda_j$, $j = 1, 2$, and replace a by $\lambda_2 a$,

$$C_{\mathscr{L}} = \begin{bmatrix} -a & -x & z & \mu_1 \overline{z} \\ -x & -b & -\mu_2 z & -\overline{z} \\ \overline{z} & -\mu_2 \overline{z} & b & \zeta_3 \\ \mu_1 z & -z & \overline{\zeta_3} & a \end{bmatrix} \ . \tag{8.6}$$

Conjugating with the unitary U given in (2.11), and replacing z by $\sqrt{2}z$, yields $\widetilde{C}_{\mathscr{L}}$, the characteristic matrix for the associated unital basis:

$$\widetilde{C}_{\mathscr{L}} = \begin{bmatrix} -x - \frac{a}{2} & (\lambda_1 - \lambda_2)\frac{a}{2} & (1-\mu_2)z & (\mu_1 - 1)\overline{z} \\ (\lambda_1 - \lambda_2)\frac{a}{2} & x - \frac{a}{2} & (1+\mu_2)z & (1+\mu_1)\overline{z} \\ (1-\mu_2)\overline{z} & (1+\mu_2)\overline{z} & \lambda_1 a & \zeta_3 \\ (\mu_1 - 1)z & (1+\mu_1)z & \overline{\zeta_3} & \lambda_2 a \end{bmatrix} \ . \tag{8.7}$$

Defining $\nu_j = \mu_j + 1$, $j = 1, 2$ and dropping the subscript on ζ_3, we have the reduced characteristic matrix

$$\widetilde{R}_{\mathscr{L}} = \begin{bmatrix} x - \frac{a}{2} & \nu_2 z & \nu_1 \overline{z} \\ \nu_2 \overline{z} & \lambda_1 a & \zeta \\ \nu_1 z & \overline{\zeta} & \lambda_2 a \end{bmatrix} \tag{8.8}$$

To break the homogeneity, let us fix $\mathrm{Tr}[R_{\mathscr{L}}] = 1$, which means $x + \frac{a}{2} = 1$. For positivity, we must have $x \geq \frac{a}{2} > 0$, and hence $0 \leq 1 \leq a$. We now determine the extreme points in the set of (a, z, ζ) for which $\widetilde{R}_{\mathscr{L}}$ is positive semidefinite.

If $a = 0$, then necessarily $z = \zeta = 0$, so $(a, z, \zeta) = (0, 0, 0)$ is extreme. If $a = 1$, then $x - \frac{a}{2} = 0$, and necessarily $z = 0$. Then extremality reduces to $|\zeta| = \sqrt{\lambda_1 \lambda_2}$. Thus,

$$(1, 0, \sqrt{\lambda_1 \lambda_2} e^{i\theta})$$

yields a one parameter family of extreme points.

Now we turn to the cases in which $0 < a < 1$. Suppose first that

$$|\zeta| = a\sqrt{\lambda_1 \lambda_2} \ . \tag{8.9}$$

As with $a = 1$, it is again the case that $z = 0$ is necessary for positivity of $R_{\mathscr{L}}$. To see this, define

$$A := \begin{bmatrix} \lambda_1 a & \zeta \\ \overline{\zeta} & \lambda_2 a \end{bmatrix} \ , \quad \vec{v} := (z\nu_2, \overline{z}\nu_1) \ , \quad \vec{\eta} := (\eta_1, \eta_2) \quad \text{and} \quad \vec{Z} := (t, \eta_1, \eta_2)$$

where $\eta_1, \eta_2 \in \mathbb{C}$ and $t \in \mathbb{R}$. Then, again with $x = 1$,

$$\langle \vec{Z}, R_{\mathscr{L}} \vec{Z} \rangle = t^2(1-a) + 2t\mathrm{Re}\left(\langle \vec{v}, \vec{\eta} \rangle\right) + \langle \vec{\eta}, A\vec{\eta} \rangle \ .$$

Minimizing over t, we find $\langle \vec{\eta}, B(z)\vec{\eta} \rangle$ where

$$B(z) := \begin{bmatrix} a\lambda_1 - \frac{|z|^2}{(1-a)}\nu_2^2 & \zeta - \frac{\overline{z}^2}{(1-a)}\nu_1\nu_2 \\ \overline{\zeta} - \frac{z^2}{(1-a)}\nu_1\nu_2 & a\lambda_2 - \frac{|z|^2}{(1-a)}\nu_1^2 \end{bmatrix} \ .$$

When (8.9) is satisfied, A has rank one, and $B(z)$ is the difference of two positive rank one matrices. Hence $B(z)$ cannot be positive definite unless the two rank one matrices are proportional. Since the null space of A is spanned by $w := (-\sqrt{\lambda_2}, \sqrt{\lambda_1}e^{i\theta})$ where $\zeta = |\zeta|e^{i\theta}$, when $y \neq 0$, it is only possible for $B(z)$ to be positive in case $\langle v, w \rangle = 0$. However, $|\langle v, w \rangle| \geq |z||\sqrt{\lambda_1}\nu_1 - \sqrt{\lambda_2}\nu_2|$, and

$$|\sqrt{\lambda_1}\nu_1 - \sqrt{\lambda_2}\nu_2| = \left(\frac{(\lambda_1, \lambda_2)_m}{\sqrt{\lambda_1\lambda_2}} - 1\right)|\sqrt{\lambda_2} - \sqrt{\lambda_1}| \ .$$

Under the assumption $\lambda_1 \neq \lambda_2$, this is non-zero unless m is the point mass at $1/2$; i.e., in the KMS case.

Thus, when (8.9) is satisfied, except in the KMS case, $z = 0$ is necessary and sufficient for the reduced characteristic matrix to be positive semidefinite. We set aside the KMS case since we already have a complete description of it for general N. Then

$$(0,0,0) \qquad \text{and} \quad (1, 0, \sqrt{\lambda_1\lambda_2}e^{i\theta}) \ , \quad 0 \leq \theta < 2\pi \ , \tag{8.10}$$

are all of the extreme points where (8.9) is satisfied. Notice that they are exactly the ones that are evenly symmetric.

Now consider pairs (a, ζ) such that $|\zeta| < a\sqrt{\lambda_1\lambda_2}$. Then $B(0) > 0$. Writing $z =: |z|e^{i\varphi}$ and holding φ fixed, there is $r_0 > 0$ such that for $|z| \leq r_0$, $B(|z|e^{i\varphi}) \geq 0$, but for $|z| > r_0$, $B(z)$ has a negative eigenvalue. It follows that a necessary condition for extremality is that $\det(B(|z|e^{i\varphi})) = 0$. Computing $\det(B(|z|e^{i\varphi})) = 0$ yields

$$r_0^2 = \frac{(1-a)(a^2\lambda_1\lambda_2 - |\zeta|^2)}{a(\lambda_1\nu_1^2 + \lambda_2\nu_2^2) - 2\nu_1\nu_2\mathrm{Re}\left(\zeta e^{i2\varphi}\right)} \ . \tag{8.11}$$

Note that the denominator in this expression is strictly positive since $|\mathrm{Re}\left(\zeta e^{i2\varphi}\right)| \leq a\sqrt{\lambda_1\lambda_2}$ and hence

$$\begin{aligned} \left(a(\nu_2^2\lambda_2 + \nu_1^2\lambda_1) - \nu_1\nu_2 2\mathrm{Re}\left(\zeta e^{i2\varphi}\right)\right) &\geq \left(a(\nu_2^2\lambda_2 + \nu_1^2\lambda_1) - 2\nu_1\nu_2 a\sqrt{\lambda_1\lambda_2}\right) \\ &= a(\nu_1\sqrt{\lambda_1} - \nu_2\sqrt{\lambda_2})^2 > 0 \ . \end{aligned}$$

Thus the remaining extreme points are those given by

$$(a, r_0 e^{i\varphi}, r\sqrt{\lambda_1\lambda_2}e^{i\theta}) \qquad 0 < a < 1\ , \quad 0 \le r < a\ , \quad 0 \le \theta, \varphi < 2\pi\ , \tag{8.12}$$

with r_0 given by (8.11).

To write $\mathscr{L}$ in the canonical form $\mathscr{L}(A) = G^*A + AG + \Phi(A)$, we easily read off from (8.7):

$$G = \begin{bmatrix} \frac{a}{4}(3\lambda_1 - \lambda_2) - \frac{x}{2} & \frac{z}{\sqrt{2}}(\mu_1 - \mu_2) \\ \frac{\overline{z}}{\sqrt{2}}(\mu_1 - \mu_2) & \frac{a}{4}(3\lambda_2 - \lambda_1) - \frac{x}{2} \end{bmatrix} + \frac{1}{\sqrt{2}}(2 - \mu_1 - \mu_2) \begin{bmatrix} 0 & z \\ -\overline{z} & 0 \end{bmatrix}\ .$$

Thus writing $G = H + iK$, H and K self-adjoint, we have that

$$K := \frac{1}{\sqrt{2}i}(2 - \mu_1 - \mu_2) \begin{bmatrix} 0 & z \\ -\overline{z} & 0 \end{bmatrix}$$

and by (8.6),

$$z = \langle u_1, \mathscr{L}(|u_1\rangle\langle u_1|)u_2\rangle\ .$$

It is easy to check that in the KMS case, this formula for K coincides with that given by Theorem 1.9. To write Φ in Kraus form amounts to diagonalizing the 3×3 matrix $R_{\mathscr{L}}$ given by (8.8). Evidently this can be done in closed form, but the resulting formulas are complicated and shed little light on matters.

9. Appendix

In this appendix we recall some ideas of Arveson that were originally developed in the context of minimal Stinespring representation, but which have, in our finite dimensional setting, a very simple expression in terms of minimal Kraus representations. This complements previous work by Choi [5]. The required background on Stinespring representations can be found in the initial chapters of [12].

Let Φ be a completely positive map on the algebra $\mathscr{A} = \mathcal{M}_N(\mathbb{C})$, and let $\Phi(A) = \sum_{j=1}^{M} V_j^* A V_j$ be a Kraus representation of it. The same data can be cast as a Stinespring representation of Φ, which was actually Kraus' starting point. Let $\mathfrak{H}_{N,M}$ denote the Hilbert space consisting of all $N \times M$ matrices X equipped with the Hilbert-Schmidt inner product. Define a representation of $\mathcal{M}_N(\mathbb{C})$ on $\mathfrak{H}_{N,M}$ by

$$\pi(A)X = AX\ . \tag{9.1}$$

Define a linear transformation $\mathcal{V} : \mathbb{C}^N \to \mathfrak{H}_{N,M}$ by

$$\mathcal{V}x = [V_1x, \dots, V_Mx] \ , \tag{9.2}$$

where $[x_1, \cdots x_M]$ denotes the $N \times M$ matrix whose jth column is x_j. Then for $X = [x_1, \cdots, x_M] \in \mathfrak{H}_{N,M}$, $\langle X, \mathcal{V}x\rangle_{\mathfrak{H}_{N,M}} = \mathrm{Tr}[[x_1, \cdots, x_M]^*[V_1x, \dots, V_Mx]] = \sum_{j=1}^{M} \langle V_j^* x_j, x\rangle$, from which it follows that

$$\mathcal{V}^* X = \sum_{j=1}^{M} V_j^* x_j \ . \tag{9.3}$$

Thus we have the Stinespring representation

$$\Phi(A) = \mathcal{V}^* \pi(A) \mathcal{V} \ , \tag{9.4}$$

in terms of a map $\mathcal{V}$ from $\mathbb{C}^N$ into some other Hilbert space, and a representation of $\mathcal{M}_N(\mathbb{C})$ on that Hilbert space. Stinespring's Theorem says that every CP map is of this form.

The Stinespring representation (9.4) is *minimal* in case the closed span of

$$\{\pi(A)\mathcal{V}x \ : \ A \in \mathscr{A} \ , \ x \in \mathbb{C}^N\}$$

is all of $\mathfrak{H}_{N,M}$, the closure being irrelevant in this finite dimensional case.

9.1 Lemma. *The Stinespring representation* (9.3) *specified by* (9.2) *is minimal if and only if* $\{V_1, \dots, V_M\}$ *is linearly independent.*

Proof. Suppose that $W = [w_1, \dots, w_M]$ is non-zero and orthogonal to $\pi(A)\mathcal{V}x$ for all $A \in \mathscr{A}$ and all $x \in \mathbb{C}^N$. Then $0 = \langle W, A\mathcal{V}x\rangle_{\mathfrak{H}_{N,M}} = \langle \mathcal{V}^* A^* W, x\rangle$, and hence the orthogonality is equivalent to the condition $\mathcal{V}^* A^* W = 0$ for all $A \in \mathscr{A}$.

Suppose that $\{V_1, \dots, V_M\}$ is not linearly independent. Then there is a non-zero vector v such that $\sum_{j=1}^{M} v_j V_j^* = 0$. Let $x \in \mathbb{C}^N$ be arbitrary, and define $W = [v_1x, \dots, v_Mx]$. Then $A^*W = [v_1A^*x, \dots, v_MA^*x]$ and $\mathcal{V}^*A^*W = \left(\sum_{j=1}^{M} v_j V_j^*\right) A^*x = 0$. Thus, there exists a non-zero $N \times M$ matrix W such that W is orthogonal to $\pi(A)\mathcal{V}x$ for all $A \in \mathscr{A}$ and all $x \in \mathbb{C}^N$, which proves the necessity of the condition.

Suppose W is a non-zero matrix such that $\mathcal{V}^*A^*W = 0$ for all $A \in \mathscr{A}$. Let r be the rank of W; evidently $0 < r \leq \min\{M, N\}$. Let $W = QR$ be a QR factorization of W so that Q is an $N \times r$ matrix with orthonormal columns and R is an $r \times M$ with linearly independent rows. Write $Q = [q_1, \dots, q_r]$, and extend $\{q_1, \dots, q_r\}$ to an orthonormal basis $\{q_1, \dots, q_N\}$ of $\mathbb{C}^N$ if $r < N$. Define an $N \times N$ matrix B by $Bq_j = q_1$ for $j \leq r$, and, in case $r < N$, $Bq_j = 0$ for $j > r$. Then $BQR = [q_1, \dots \ , q_1]R$;

i.e., $(BQR)_{i,j} = (q_1)_i \sum_{k=1}^{r} R_{k,j}$. Since the rows of R are linearly independent, the vector $v \in \mathbb{C}^M$ with $v_j = \sum_{k=1}^{r} R_{k,j}$ is not zero. Hence for any $w \in \mathbb{C}^N$, taking $A^* = UB$ where U is an appropriate chosen unitary, we can arrange that $A^*W = [v_1 w, \dots, v_M w]$, and then

$$0 = \mathcal{V}^* A^* W = \left(\sum_{j=1}^{M} v_j V_j^* \right) w \ ,$$

and since w is arbitrary, this implies that $\sum_{j=1}^{M} v_j V_j^* = 0$. This is impossible since $\{V_1, \dots, V_m\}$ are linearly independent, and hence W must be zero. This proves the sufficiency of the condition. □

The next theorems involve maps of the form

$$\Psi(A) = \sum_{i,j=1}^{M} B_{i,j} V_i^* A V_j \tag{9.5}$$

where $\{V_1, \dots, V_M\} \subset \mathscr{A}$, and B is an $M \times M$ matrix. Suppose that B is positive so that $B = S^*S$. Then writing $B_{i,j} = \sum_{k=1}^{M} S_{i,k}^* S_{k,j} = \sum_{k=1}^{M} \overline{S_{k,i}} S_{k,j}$,

$$\Psi(A) = \sum_{k=1}^{M} W_k^* A W_k \quad \text{where} \quad W_k = \sum_{j=1}^{M} S_{k,j} V_j \ .$$

It follows that whenever $B \geq 0$, Ψ is CP, and this is true without any hypotheses on $\{V_1, \dots, V_M\}$.

Now suppose that $\{V_1, \dots, V_M\}$ is linearly independent. The Gram-Schmidt procedure yields an orthonormal set $\{E_1, \dots, E_M\}$ and an invertible lower triangular matrix L such that $V_i = \sum_{j=1}^{M} L_{i,j} E_j$. Then

$$\Psi(A) = \sum_{i,j=1}^{M} B_{i,j} V_i^* A V_j = \sum_{i,j,k,\ell=1}^{M} B_{i,j} \overline{L_{i,k}} E_k^* A L_{j,\ell} E_\ell = \sum_{k,\ell=1}^{M} (L^* B L)_{i,j} E_k^* A E_\ell \ .$$

Since $\{E_1, \dots, E_M\}$ is orthonormal, Ψ is CP if and only if L^*BL is positive semidefinite. But since L is invertible, this is the case if and only if B is positive semidefinite. Moreover, we see that there is at most one matrix B for which Ψ can be written in the form (9.5) since L^*BL is the characteristic matrix of Ψ for an orthonormal basis determined by $\{V_1, \dots, V_M\}$. This proves:

9.2 Lemma. *Let Ψ be a map defined by (9.5) for some set $\{V_1, \dots, V_M\} \subset \mathcal{M}_N(\mathbb{C})$ and some $M \times M$ matrix B. Then if B is positive semi-definite, Ψ is CP, and if $\{V_1, \dots, V_M\}$*

is linearly independent, Ψ is CP if and only if B is positive semi-definite, and in this case the correspondence between Ψ and B is one-to-one.

Now let Φ and Ψ be two CP maps. Then $\Phi - \Psi$ is CP if and only if $C_\Phi - C_\Psi \geq 0$. Thus, the invertible transformation $\Phi \mapsto C_\Phi$ identifies the order structure on $CP(\mathscr{A})$ with the order structure on $\mathcal{M}_N(\mathbb{C})^+$, the positive semidefinite elements of $\mathcal{M}_N(\mathbb{C})$. There is another characterization of this order relation due to Arveson that has several advantages.

9.3 Theorem. *Let Φ be a completely positive map given by a minimal Kraus representation $\Phi(A) = \sum_{j=1}^M V_j^* A V_j$. Then a CP map Ψ satisfies $\Phi \geq \Psi$ if and only if there is a uniquely determined $M \times M$ matrix T such that $0 \leq T \leq \mathbf{1}$ and*

$$\Psi(A) = \sum_{i,j=1}^M T_{i,j} V_i^* A V_j \ . \tag{9.6}$$

Equivalently, in terms of the associated minimal Stinespring representation $\Phi(A) = \mathcal{V}^* \pi(A) \mathcal{V}$, there is a positive operator $\widetilde{T} \in \pi(\mathcal{M}_N(\mathbb{C}))'$, the commutant of $\pi(\mathcal{M}_N(\mathbb{C}))$, such that

$$\Psi(A) = \mathcal{V}^* \pi(A) \widetilde{T} \mathcal{V} \ . \tag{9.7}$$

9.4 Remark. Arveson [2, Theorem 1.4.2] proved the theorem in the second equivalent form, and discussed it as being a non-commutative Radon-Nikodym Theorem with the Radon-Nikodym derivative being the element $\widetilde{T}$ of $\pi(\mathcal{M}_N(\mathbb{C}))'$.

Proof. Let T be an $M \times M$ matrix, with $0 \leq T \leq \mathbf{1}$, and let $\Psi(A)$ be given by (9.6). Since $T \geq 0$, Ψ is CP by Lemma 9.2, and

$$\Phi(A) - \Psi(A) = \sum_{i,j=1}^M (\delta_{i,j} - T_{i,j}) V_i^* A V_j \ .$$

Since $\mathbf{1} - T \geq 0$, by another application of Lemma 9.2, $\Phi - \Psi$ is CP.

Conversely, suppose that $\Phi - \Psi$ is CP. We again use the Gram-Schmidt procedure to produce an orthonormal set $\{E_1, \ldots, E_M\}$ and an invertible lower triangular matrix T such that $V_i = \sum_{j=1}^M L_{i,j} E_j$. Then $\Phi(A) = \sum_{j=1}^M (L^* L)_{i,j} E_i^* A E_j$.

If $M < N^2$, extend $\{E_1, \ldots, E_M\}$ to an orthonormal basis of $\mathcal{M}_N(\mathbb{C})$ equipped with the Hilbert-Schmidt inner product. The characteristic matrix of Φ with respect to this basis, C_Φ, has $L^* L$ as its upper-left $M \times M$ block, and all other entries are zero. If Ψ is a CP map such that $\Phi - \Psi$ is CP, then $C_\Phi - C_\Psi$ is positive semidefinite. Hence for some $M \times M$ matrix R with $0 \leq R \leq L^* L$, $\Psi(A) = \sum_{i,j=1}^M R_{i,j} E_i^* A E_j$. But then since $E_j = \sum_{k=1}^M L_{j,k}^{-1} V_k$,

$$\Psi(A) = \sum_{i,j=1}^{M} ((L^{-1})^* R L^{-1})_{i,j} E_i^* A E_j \ .$$

Since $0 \leq R \leq L^*L$, $0 \leq (L^{-1})^* R L^{-1} \leq \mathbf{1}$. Hence we may define $T := (L^{-1})^* R L^{-1}$ and we have the contraction. This completes the proof that a CP map Ψ satisfies $\Psi \leq \Phi$ if and only if Ψ has the form specified in (9.6).

We now show that this is equivalent to Ψ having the form specified in (9.7). For an $N \times M$ matrix X and an $M \times M$ matrix B, define

$$\pi'(B)X = XB^{\mathrm{T}} \ ,$$

where B^{T} denotes the transpose of B. It is easy to check that π' is a $*$-representation of $M_M(\mathbb{C})$ on $\mathfrak{H}_{N,M}$. It is immediately clear that $\pi'(M_M(\mathbb{C}))$ lies in the commutant of $\pi(\mathcal{M}_N(\mathbb{C}))$ since π' acts by right multiplication, and π acts by left multiplication, and it is easy to check that in fact $(\pi(\mathscr{A}))' = \pi'(M_M(\mathbb{C}))$.

Now write $X \in \mathfrak{H}_{N,M}$ in the form $X = [x_1, \dots, x_M]$. Then for any $M \times M$ matrix R

$$\sum_{j=1}^{M} [R_{1,j}x_j, \dots, R_{M,j}x_j] = XR^{\mathrm{T}} \ .$$

Suppose now that Ψ has the form specified in (9.6). Then for all $x, y \in \mathbb{C}^N$,

$$\langle x, \Psi(A)y\rangle = \sum_{i=1}^{M} \langle V_i x, A \sum_{j=1}^{M} T_{i,j} V_j y\rangle = \langle x, \mathcal{V}^* \pi(A) \pi'(T^{\mathrm{T}}) \mathcal{V} y\rangle \ .$$

Defining $\widetilde{T} := \pi'(T^{\mathrm{T}})$, we obtain (9.7).

Finally, assume that Ψ has the form (9.7). Since $\pi(\mathscr{A})' = \pi'(M_M(\mathbb{C}))$ we can write $\widetilde{T} = \pi'(T^{\mathrm{T}})$ for some $M \times M$ matrix T with $0 \leq T \leq 1$. Then

$$\Psi(A) = \mathcal{V}^* \pi(A) \widetilde{T} \mathcal{V} = \Psi(A) = \mathcal{V}^* \pi(A) \pi'(T^{\mathrm{T}}) \mathcal{V} = \mathcal{V}^* \pi(A) \mathcal{W}$$

where

$$\mathcal{W}x = [W_1 x, \dots, W_M x] \qquad \text{and} \qquad W_i = \sum_{j=1}^{M} T_{i,j} V_j \ .$$

Then Ψ has the form specified in (9.6) □

We now turn to a question addressed by Arveson: A CP map is *unital* in case $\Phi(\mathbf{1}) = \mathbf{1}$. Evidently the set of unital CP maps is convex. An element Φ of this convex set is extremal in case whenever Ψ is another unital CP map such that for some $t \in (0,1)$, $t\Psi \leq \Phi$, then

necessarily $\Psi = \Phi$. What are necessary and sufficient conditions for a unital CP map Φ to be extremal in the cone of unital CP maps?

Arveson's answer is stated in terms of minimal Stinespring representations and the commutant of $\pi(\mathcal{M}_N(\mathbb{C}))$, where π is the representation in the Stinespring representation. In our finite dimensional setting, there is a much simpler expression, due to Choi, of this condition in terms of a minimal Kraus representation:

9.5 Theorem. *Let Φ be a unital CP map with a minimal Kraus representation $\Phi(A) = \sum_{j=1}^{M} V_j^* A V_j$. In order for Φ to be extremal in the cone of unital CP maps, it is necessary and sufficient that the M^2 matrices*

$$\{\ V_i^* V_j\ :\ 1 \le i,j \le M\ \} \tag{9.8}$$

are linearly independent.

9.6 Remark. Choi [5, Theorem 5] gave an elementary proof of this result that bypasses the use of Arveson's Radon-Nikodym Theorem. We give a very short matricial rendering of Arveson's original proof [2, Theorem 1.4.6] using Theorem 9.3. It is worth noting, as Arveson did, that the proof applies, and yields the same result, if applied to the class of CP maps for which $\Phi(\mathbf{1}) = K$, for any fixed $0 \le K \le \mathbf{1}$.

Proof. Suppose first that the set in (9.8) is linearly independent. Let Ψ be CP and unital with $t\Psi \le \Phi$ for some $0 < t < 1$. Then by Theorem 9.3, there is an $M \times M$ matrix T with $0 \le T \le \mathbf{1}$ such that

$$t\Psi(A) = \sum_{i,j=1}^{M} T_{i,j} V_i^* A V_j\ .$$

Taking $A = \mathbf{1}$, we get $t\mathbf{1} = \sum_{i,j=1}^{M} T_{i,j} V_i^* V_j$, and then since $t\mathbf{1} = t\Phi(\mathbf{1}) = \sum_{j=1}^{M} t V_j^* V_j$, we have $\sum_{i,j=1}^{M} B_{i,j} V_i^* V_j = 0$ where $B_{i,j} = t\delta_{i,j} - T_{i,j}$. By the linear independence, $B_{i,j} = 0$ for each i,j, and hence $T = t\mathbf{1}$. Thus $t\Psi = t\Phi$, and so Φ is extreme.

For the converse, suppose that Φ is extreme. The set in (9.8) is linearly independent if and only if the map $B \mapsto \sum_{i,j} B_{i,j} V_i^* V_j$ is injective. Because this map is Hermitian, to show that it is injective, it suffices to show that it is injective on the self-adjoint $M \times M$ matrices. Therefore, consider a self-adjoint B such that $\sum_{i,j} B_{i,j} V_i^* V_j = 0$. Replacing B with a positive multiple of itself, we may freely assume that $\|B\| \le 1$. Define $T = \frac{1}{2}(\mathbf{1} + B)$, and then define Ψ by $\Psi(A) = \sum_{i,j=1}^{M} T_{i,j} V_i^* V_j$. Ψ is CP with $\Psi \le \Phi$ by Theorem 9.3, and $\Psi(\mathbf{1}) = \frac{1}{2}\mathbf{1}$ since $\sum_{i,j} B_{i,j} V_i^* V_j = 0$. Therefore, defining $\widetilde{\Psi} = 2\Psi$, we have that $\widetilde{\Psi}$ is unital, CP, and $\frac{1}{2}\widetilde{\Psi} \le \Phi$. Since Φ is extreme, $\widetilde{\Phi} = \Phi$, and hence $2T = \mathbf{1}$ and $B = 0$. □

Declaration of competing interest

There is no competing interest.

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