1. Introduction

If J is an open subinterval of $\mathbb{R}$ and f is a real-valued function defined on J then for each self-adjoint operator A on a finite-dimensional complex inner product space, the spectrum of which is contained in J, there is defined a self-adjoint operator which is denoted by $f(A)$. One refers to the "operator function" f. If J and J' are open subintervals of $\mathbb{R}$ and F is a real-valued function of two variables defined on $J \times J'$ then for each pair A, B of self-adjoint operators on finite-dimensional complex inner product spaces X and Y respectively, with spectra contained in J and J' respectively, there is defined a self-adjoint operator $F(A, B)$ on the tensor product space $X \otimes Y$. One refers to the "operator function" F of two variables.

There is a substantial literature concerning these operator functions and their properties. A function $f : J \to \mathbb{R}$ is said to be *operator monotone* if $f(A) \leq f(B)$ whenever the terms are defined and $A \leq B$. There is also a natural concept of *operator convexity* which for functions of one variable is intimately related to operator monotonicity. (Formal definitions are given in subsequent sections.) The present paper is concerned with the Fréchet differentiability and operator convexity of operator functions.

In 1934 Löwner [13], in a celebrated paper, characterised those functions $f : J \to \mathbb{R}$ which are operator monotone; they are, in particular, analytic. Several proofs of Löwner's central result are presented in a monograph by Donoghue [5]. More recently Hansen and Pedersen [9] have obtained yet another and very interesting proof and their development is followed in [4]. Part I of this paper is in part a response to their paper; it prompted the present authors to ask to what extent the results of the theory of operator monotone and operator convex functions can be obtained by exploiting the calculus. Theorems 2.1 and 4.2 include the results that, in both the one and two-variable situations, if a real-valued function is continuously L times differentiable then the associated operator functions are L times Fréchet differentiable with continuous Fréchet derivatives. These theorems fill a longstanding gap in the theory. They allow straightforward and direct uses of the calculus in contexts where in the past ad hoc substitutes for the calculus have often been used. In particular the elementary differential conditions for monotonicity and convexity of real-valued functions extend naturally to operator functions (Theorems 3.1 and 3.2). Theorems 4.2 and 3.2 are exploited in Part II of the paper. Matrix forms of these results, previously obtained in the two-variable case by relatively ad hoc methods, follow immediately. The Fréchet differentiability of operator functions on infinite-dimensional Hilbert spaces is the subject of a paper by Hansen and Pedersen [8] but the overlap with the present paper is very slight. (Readers are referred to [6] for a systematic presentation of the Fréchet differential calculus and for the notation which we use.)

The most novel result in Part I is Theorem 2.5 in which the operator functions corresponding to a continuously differentiable function $f : J \to \mathbb{R}$ are expressed *algebraically* in terms of their (first) Fréchet derivatives.

Part II of the paper is concerned with operator convex functions of two variables. Operator convex functions of one variable were characterised by Bendat and Sherman [3]; an alternative and elegant treatment is given in [9]. Little has been known about operator convex functions of two variables. The one-variable developments in [3] and [9] both exploit the relation between operator monotonicity and operator convexity for which there is no two-variable analogue.

Let $\mathcal{OC}_1$ denote the set of operator convex functions $f : (-1,1) \to \mathbb{R}$; it is a convex cone. A function $f : (-1,1) \to \mathbb{R}$ is in $\mathcal{OC}_1$ if and only if it has an integral representation

$$f(s) = f(0) + f'(0)s + \frac{1}{2}f''(0)\int \frac{s^2}{1-\alpha s}\, dM(\alpha)$$

for some (unique) probability measure M on $[-1,1]$ (stated as Thm. 5.1). The cone $\mathcal{OC}_1$ has a *base* $\mathcal{K}_1$ (defined by $f(0) = f'(0) = 0,\ f''(0) = 2$) and its set of extreme points is the topological interval of functions $s^2(1-\alpha s)^{-1}$, $\alpha \in [-1,1]$.

Let $\mathcal{OC}_2$ be the set of operator convex functions $f : (-1,1)^2 \to \mathbb{R}$. It is a convex cone. It is known [2] that if $|\alpha| \le 1, |\beta| \le 1$ then $f(s,t) = (1-\alpha s)^{-1}(1-\beta t)^{-1} \in \mathcal{OC}_2$ (see Section 4). These are functions which in each variable separately are "extremal" in the convex cone $\mathcal{OC}_1$. The investigation in Part II stems from this fact. Any such function has representations

$$f(s,t) = \lambda(s) + \mu(s)t + \nu(s)\frac{t^2}{1-\beta(s)t}$$

and

$$f(s,t) = l(t) + m(t)s + n(t)\frac{s^2}{1-\alpha(t)s}.$$

These equations are solved in Section 6 under the assumption that the functions $\alpha(t)$ and $\beta(s)$ have continuous second derivatives: if f is such a function then for some $(\alpha,\beta,e) \in \mathbb{R}^3$ satisfying the inequalities

$$|\alpha+\beta| - 1 \le e \le 1 - |\alpha-\beta|, \tag{1.1}$$

(which implies that $|\alpha| \le 1,\ |\beta| \le 1$), f must be of the form

$$f(s,t) = A + Bs + Ct + \frac{\Delta st + \Sigma_0 s^2 + \Gamma_0 t^2 + \Sigma_1 s^2 t + \Gamma_1 t^2 s + G s^2 t^2}{1 - \alpha s - \beta t + est} \tag{1.2}$$

(Thm. 6.5 and Prop. 6.2). It is an open question whether the smoothness assumption is redundant.

Let $F(\alpha,\beta,e)$ be the set of functions of this form which are operator convex; it is a face of the convex cone $\mathcal{OC}_2$ (Thm. 6.4).

Functions $f : (-1,1)^2 \to \mathbb{R}$ given by (1.2), subject to (1.1), are infinitely differentiable and so, by Thm. 4.2, their operator functions are infinitely Fréchet differentiable. In Section 7 their second Fréchet derivatives (more precisely, the operators $d^2f(A,B)(H,K)^2 \in \mathcal{S}(\mathbb{C}^M \otimes \mathbb{C}^N)$) are calculated. The calculations are not entirely straightforward; a simple power series expansion of $f(A+H, B+K)$ involves products in the algebra of operators on $\mathbb{C}^M \otimes \mathbb{C}^N$ and yields a formula for $d^2f(A,B)(H,K)^2$ which is not apparently self-adjoint. It is a non-trivial matter to find and establish a tractable form for $d^2f(A,B)(H,K)^2$. This is done in Thm. 7.1, and in Thm. 7.2 the differential criterion for convexity, of Thm. 3.2, is used to characterise those functions of the form (1.2) which are operator convex: the function must be convex on $(-1,1)^2$ and the coefficients in (1.2) must satisfy the equations

$$\Sigma_0 e + \Sigma_1 \alpha = \Gamma_0 + \Gamma_1 \beta = G = 0.$$

This characterisation permits a detailed analysis in Section 8 of the faces $F(\alpha,\beta,e)$ of the cone $\mathcal{OC}_2$. The analysis is not entirely complete but a considerable amount of information is obtained. Thm. 8.1 is concerned with the set of $(\alpha,\beta,e) \in \mathbb{R}^3$ for which the face $F(\alpha,\beta,e)$ is non-trivial, i.e. of dimension greater than three. For each $(\alpha,\beta) \in [-1,1]^2$ the set $\{e : \dim F(\alpha,\beta,e) > 3\}$ is closed and non-empty and contains a non-trivial interval unless either $\max\{|\alpha|,|\beta|\} = 1$ or $\alpha\beta = 0$, in which cases the set is the single point $\alpha\beta$. However the description of these sets is not yet complete.

The cone $\mathcal{OC}_2$ has a natural closed convex *base* $\mathcal{K}_2$ (see Prop. 5.3). (It is an important open question whether $\mathcal{K}_2$ is compact.) Thm. 8.2 states that the intersections of the faces $F(\alpha,\beta,e) \cap \mathcal{K}_2$ of $\mathcal{K}_2$ are almost all empty, the non-empty intersections being single extreme points of $\mathcal{K}_2$. Thm. 8.3 establishes that a face $F(\alpha,\beta,e)$ of $\mathcal{OC}_2$ is of dimension 3, 4, 6, 7 or 8, and that all these cases occur.

Theorem 8.4 is concerned with the set of extreme points of $F(\alpha,\beta,e) \cap \mathcal{K}_2$, which can be determined in most, possibly all, cases. The typical cases are those in which $\dim F(\alpha,\beta,e) = 6$. If, considering the first (α,β)-quadrant, $0 < \alpha < 1$, $0 < \beta < 1$ and $\max\{0, \alpha+\beta-1\} \le e \le \alpha\beta$ then $\dim F(\alpha,\beta,e) = 6$ and $F(\alpha,\beta,e) \cap \mathcal{K}_2$ is a two-dimensional convex set; if also $\alpha+\beta-1 < e$ then each point of the relative boundary is an extreme point of $\mathcal{K}_2$. Thus $\operatorname{ext}\mathcal{K}_2$ contains four (one for each (α,β)-quadrant) disjoint families of pairwise disjoint topological circles, each family indexed by the points (α,β,e) of a non-empty open subset of $\mathbb{R}^3$. The results provide a sharp contrast with the one-variable situation and disappoint any expectation there may have been that operator convex functions of two variables might have a characterisation analogous in a straightforward way to the characterisation of operator convex functions of one variable.

I. THE CALCULUS

2. Operator functions of one variable

For a positive integer N let $\mathbb{C}^N$ be the standard N-dimensional complex linear space equipped with its natural inner product $\langle\cdot,\cdot\rangle$. The natural coordinate system of $\mathbb{C}^N$ will play no role. Let $\mathcal{L}(\mathbb{C}^N)$ denote the space of linear operators on $\mathbb{C}^N$ and let $\mathcal{S}(\mathbb{C}^N) = \mathcal{S}$ be the real linear space of self-adjoint operators defined on $\mathbb{C}^N$. If J denotes a subinterval (usually open) of $\mathbb{R}$ let $\mathcal{S}_J(\mathbb{C}^N) = \mathcal{S}_J$ denote the set of operators in $\mathcal{S}$ with spectrum contained in J. If J is open then $\mathcal{S}_J$ is a convex open subset of $\mathcal{S}$.

DEFINITION. To each real-valued function $f : J \to \mathbb{R}$ defined on J there corresponds an *operator function* $f : \mathcal{S}_J \to \mathcal{S}$ defined in the following way. An operator $A \in \mathcal{S}_J$ has a spectral decomposition

$$A = \sum \lambda_k E_k \tag{2.1}$$

in which $\lambda_1, \lambda_2, \ldots$ are the distinct eigenvalues of A and $E_1, E_2, \ldots$ are the corresponding orthogonal projections onto eigenspaces of A. An operator, denoted by $f(A)$, in $\mathcal{S}$ is defined by

$$f(A) = \sum_{k=1}^{n} f(\lambda_k) E_k.$$

If $N = 1$ then $f(\lambda I)$ (where I denotes the identity operator) can be identified with $f(\lambda)$. It is natural to regard the operator functions f (one for each integer N) as extensions of $f : J \to \mathbb{R}$ and to use the same symbol for all. However it will be convenient to denote an operator function f also by Of and to think in terms of the mapping O.

The first theorem asserts that Of inherits differentiability properties from f. Let $C(J) = C^0(J)$ denote the space of continuous functions $f : J \to \mathbb{R}$. For any positive integer L let $C^L(J)$ denote the space of functions $f \in C(J)$ such that the derivative $f^{(L)}$ exists and is continuous on J. Then for each $L \geq 0$ the space $C^L(I)$ is a Fréchet space [16]. If X and Y are real normed linear spaces and Ω is an open subset of X then for each integer $L \geq 0$ we denote the space of functions $F : \Omega \to Y$ such that F and its Fréchet derivatives $dF, \ldots, d^L F$ exist and are continuous on Ω by $C^L(\Omega, Y)$. If X is a finite-dimensional space and Y is a Banach space then $C^L(\Omega, Y)$ is a Fréchet space with respect to the topology defined by the seminorms

$$\|d^l F\|_K = \sup_{x \in K} \|d^l F(x)\|,$$

where $0 \leq l \leq L$ and K is a compact subset of Ω. This fact can be proved by an extension of an elementary proof of the special case in which $X = Y = \mathbb{R}$. The extension depends upon basic results of the Fréchet differential calculus for which we refer to [6]. Our first concern is with the case $X = Y = \mathcal{S}(\mathbb{C}^N)$ and $\Omega = \mathcal{S}_J(\mathbb{C}^N)$. In this case the topology is determined by the seminorms

$$\|d^l F\|_{\mathcal{S}_{J'}} = \sup_{A \in \mathcal{S}_{J'}} \|d^l F(A)\|$$

where $0 \leq l \leq L$ and J' is a closed subinterval of J.

The lth divided difference of a function $f \in C^l(J)$ on points $\lambda_0, \ldots, \lambda_l$ (not necessarily distinct) will be denoted by $f^{[l]}(\lambda_0, \ldots, \lambda_l)$. We refer to [5] for information concerning divided differences.

The case $L = 1$ of the first theorem is largely contained in [5] (p. 79). The case $L = 2$ is in part contained, in matrix form, in [11].

THEOREM 2.1. *Let $f \in C^L(J)$, where $L \geq 0$. Then $Of \in C^L(\mathcal{S}_J, \mathcal{S})$. The mapping $O : C^L(J) \to C^L(\mathcal{S}_J, \mathcal{S})$ is continuous.*

If $f \in C^L(J), A \in \mathcal{S}_J$ and $e_1, \dots, e_N$ is an orthonormal basis of $\mathbb{C}^N$ consisting of eigenvectors of A corresponding to eigenvalues $\lambda_1, \dots, \lambda_N$ then, for $1 \leq l \leq L$, the matrix of $d^l f(A)(H_1, \dots, H_l)$ with respect to this basis is given by

$$(2.2) \qquad \langle d^l f(A)(H_1, \dots, H_l) e_{j_l}, e_{j_0} \rangle = \sum_{1 \leq j_1, \dots, j_{l-1} \leq N} f^{[l]}(\lambda_{j_0}, \dots, \lambda_{j_l}) \Big(\sum_{\sigma \in S_l} \prod_{r=1}^{l} \langle H_{\sigma(r)} e_{j_r}, e_{j_{r-1}} \rangle \Big)$$

for all $j_0, j_l \in \{1, \dots, N\}$, where S_l denotes the symmetric group of permutations of $\{1, \dots, l\}$, and the outer summation is omitted in the case $l = 1$.

If $A \in \mathcal{S}_J$ and $\mathrm{sp}(A) \subseteq J'$, where J' is a closed subinterval of J, then, for $0 \leq l \leq L$,

$$(2.3) \qquad \|d^l f(A)\| \leq N^l l! \|d^l f\|_{J'}.$$

The result will be proved first for polynomial functions and will then be extended by continuity to all of $C^L(J)$. The operator O is linear so we begin by considering the monomials $p_k \in C^\infty(\mathbb{R})$ defined for $k = 0, 1, \dots$ by $p_k(t) = t^k$. It is easily seen from the definition of $p_k(A)$ that $p_k(A) = A^k$ for all $A \in \mathcal{S}$. We can regard Op_k as a mapping of $\mathcal{L}(\mathbb{C}^N)$ into itself. The space $\mathcal{L}(\mathbb{C}^N)$ is a complex Banach algebra.

Lemma 2.2. *Let $\mathcal{A}$ be a Banach algebra and let $k \in \mathbb{N}$. Then the mapping $p_k : \mathcal{A} \to \mathcal{A}$, defined by*

$$p_k(A) = A^k$$

for all $A \in \mathcal{A}$, has Fréchet derivatives of all orders given, for $l \geq 1$, by

$$(2.4) \qquad d^l p_k(A)(H_1, \dots, H_l) = \sum_{\sigma \in S_l} \sum_{r_1 + \dots + r_{l+1} = k - l} A^{r_1} H_{\sigma(1)} A^{r_2} H_{\sigma(2)} \dots A^{r_l} H_{\sigma(l)} A^{r_{l+1}}$$

(*where, in the summation, $0 \leq r_1, \dots, 0 \leq r_{l+1}$*).

Proof. First note that

$$(2.5) \qquad p_k(A + tH) = (A + tH)^k = \sum_{l=0}^{k} t^l \Big(\sum_{r_1 + \dots + r_{l+1} = k - l} A^{r_1} H A^{r_2} H \dots A^{r_l} H A^{r_{l+1}} \Big)$$

A direct calculation now shows that $p_k : \mathcal{A} \to \mathcal{A}$ is Fréchet differentiable and that dp_k is given by (2.4) with $l = 1$.

We now outline a proof by induction that: *$d^l p_k$ exists for each $l \geq 1$ and the value $d^l p_k(A)(H_1, \dots, H_l)$ can be expressed as a finite sum of terms each of the form*

$$(2.6) \qquad T(A)(H_1, \dots, H_l) = A^{r_1} H_{\sigma(1)} A^{r_2} H_{\sigma(2)} \dots A^{r_l} H_{\sigma(l)} A^{r_{l+1}}$$

where $0 \leq r_1, \dots, 0 \leq r_{l+1}, r_1 + \dots + r_{l+1} = k - l$ and $\sigma \in S_l$. We have seen that this statement is true in the case $l = 1$.

Let $M_{\mathrm{L}} : \mathcal{A} \to \mathcal{L}(\mathcal{A})$ and $M_{\mathrm{R}} : \mathcal{A} \to \mathcal{L}(\mathcal{A})$ denote left and right multiplication; that is, for each $A \in \mathcal{A}$,

$$M_{\mathrm{L}}(A)(x) = Ax, \qquad M_{\mathrm{R}}(A)(x) = xA$$

for all $x \in \mathcal{A}$. Then M_{L} and M_{R} are linear and Fréchet differentiable. The mapping

$$T : \mathcal{A} \to \mathcal{L}_l(\mathcal{A}, \mathcal{A})$$

into the space of multilinear mappings of $\mathcal{A}^l$ into $\mathcal{A}$ defined by (2.6) can be regarded as a composite

$$\mathcal{A} \xrightarrow{\phi_1} \mathcal{A}^{l+1} \xrightarrow{\phi_2} \mathcal{L}(\mathcal{A},\mathcal{A})^l \xrightarrow{\phi_3} \mathcal{L}_l(\mathcal{A},\mathcal{A})$$

in which

$$\phi_1(A) = (A^{r_1},\dots,A^{r_{l+1}}),$$

$$\phi_2(B_1,\dots,B_{l+1}) = (M_{\mathrm{L}}(B_1),\dots,M_{\mathrm{L}}(B_{l-1}), M_{\mathrm{R}}(B_{l+1})\circ M_{\mathrm{L}}(B_l)),$$

$$\phi_3(T_1,\dots,T_l)(H_1,\dots,H_l) = T_1H_1\dots T_lH_l.$$

Elementary arguments show that ϕ_1, ϕ_2 and ϕ_3 are all Fréchet differentiable. (For example, ϕ_3 is shown to have continuous partial Fréchet derivatives and so ([6], p. 197) is differentiable.) Thus T is Fréchet differentiable.

Now

$$\begin{aligned} &dT(A)(H_{l+1})(H_1,\dots,H_l)\\ &\qquad= \frac{d}{dt}T(A+tH_{l+1})(H_1,\dots,H_l)\bigg|_{t=0}\\ &\qquad= \frac{d}{dt}(A+tH_{l+1})^{r_1}H_{\sigma(1)}\dots(A+tH_{l+1})^{r_l}H_{\sigma(l)}(A+tH_{l+1})^{r_{l+1}}\bigg|_{t=0}. \end{aligned}$$

The last term is the coefficient of t in the expansion of the product as a polynomial in t, which is a finite sum of the form (2.6) (with l replaced by $l+1$). The italicised statement above now follows by induction.

It remains to identify the derivatives d^lp_k. Let $D^{(l)}p_k(A)(H_1,\dots,H_l)$ be the right hand side of (2.4). Then $D^{(l)}p_k$ is a mapping of $\mathcal{A}$ into $\mathcal{L}_l(\mathcal{A},\mathcal{A})$. For each $A\in\mathcal{A}$ both $d^lp_k(A)$ and $D^{(l)}p_k(A)$ are symmetric multilinear mappings of $\mathcal{A}^l$ into $\mathcal{A}$. Now, for all $H\in\mathcal{A}$,

$$\begin{aligned} d^lp_k(A)(H,\dots,H) &= \frac{d^l}{dt^l}p_k(A+tH)\bigg|_{t=0} = \frac{d^l}{dt^l}(A+tH)^k\bigg|_{t=0}\\ &= l! \sum_{r_1+\dots+r_{l+1}=k-l} A^{r_1}H\dots A^{r_l}HA^{r_{l+1}}\\ &= D^{(l)}p_k(A)(H,\dots,H) \end{aligned}$$

(the first equation is by 3.6.1 of [6], the second and third terms on the right are, by (2.5), both $l!$ times the coefficient of t^l in the expansion of $(A+tH)^k$ as a polynomial in t). It follows that $d^lp_k(A) = D^{(l)}p_k(A)$. The proof of Lemma 2.2 is complete.

If we now apply Lemma 2.2 to $\mathcal{A} = \mathcal{L}(\mathbb{C}^N)$ and consider the restriction $p_k|\mathcal{S}(\mathbb{C}^N)$ we conclude that the operator function $p_k : \mathcal{S}(\mathbb{C}^N) \to \mathcal{S}(\mathbb{C}^N)$ is infinitely Fréchet differentiable with derivatives given by equation (2.4).

Now suppose that $A\in\mathcal{S}$ and that $e_1,\dots,e_N$ and $\lambda_1,\dots,\lambda_N$ are as in the statement of the theorem. Then it follows from (2.4) that

$$\begin{aligned} &\langle d^lp_k(A)(H_1,\dots,H_l)e_{j_l}, e_{j_0}\rangle\\ &\qquad= \sum_{1\le j_1,\dots,j_{l-1}\le N}\Big(\sum_{r_1+\dots+r_{l+1}=k-l}\prod_{m=0}^{l}\lambda_{j_m}^{r_{m+1}}\Big)\Big(\sum_{\sigma\in S_l}\prod_{m=1}^{l}\langle H_{\sigma(m)}e_{j_m}, e_{j_{m-1}}\rangle\Big). \end{aligned}$$

The equation (2.2) in the case $f = p_k$ now follows from the next lemma.

LEMMA 2.3. *For all* $\lambda_1, \ldots, \lambda_{l+1}$,

$$p_k^{[l]}(\lambda_1, \ldots, \lambda_{l+1}) = \sum_{r_1+\ldots+r_{l+1}=k-l} \lambda_1^{r_1} \ldots \lambda_{l+1}^{r_{l+1}}. \tag{2.7}$$

PROOF. The divided differences of an analytic function have integral representations ([5], p. 2) which for the monomial p_k can be written as

$$p_k^{[l]}(\lambda_1, \ldots, \lambda_{l+1}) = \frac{1}{2\pi i} \int_\Gamma \frac{\zeta^k}{\prod_{r=1}^{l+1}(\zeta - \lambda_r)} \, d\zeta,$$

where Γ is a (large) circle containing all of $\lambda_1, \ldots, \lambda_{l+1}$. Let $K = k - l$. Then

$$\frac{1}{\zeta - \lambda_r} = \frac{1}{\zeta}\left(1 + \frac{\lambda_r}{\zeta} + \ldots + \frac{\lambda_r^K}{\zeta^K} + \frac{\lambda_r^{K+1}}{\zeta^K(\zeta - \lambda_r)}\right).$$

Let

$$G_r = 1 + \frac{\lambda_r}{\zeta} + \ldots + \frac{\lambda_r^K}{\zeta^K}, \qquad R_r = \frac{\lambda_r^{K+1}}{\zeta^K(\zeta - \lambda_r)}.$$

Then

$$\frac{\zeta^k}{\prod_{r=1}^{l+1}(\zeta - \lambda_r)} = \zeta^{k-l-1} \prod_{r=1}^{l+1} (G_r + R_r) = \zeta^{k-l-1} \Big(\prod_{r=1}^{l+1} G_r + R \Big)$$

where R is a finite sum of $2^{l+1} - 1$ terms, each a product of $l + 1$ factors at least one of which is one of $R_1, \ldots, R_{l+1}$. If $\Lambda = \max |\lambda_r|$ and $|\zeta| \geq 2\Lambda$ then $|G_r| < 2$ and

$$|R_r| \leq \frac{2\Lambda^{K+1}}{|\zeta|^{K+1}}.$$

Therefore

$$|R(\zeta)| \leq (2^{l+1} - 1)2^l \frac{2\Lambda^{K+1}}{|\zeta|^{K+1}}.$$

Now let Γ be a circle with centre 0 and radius $\varrho \geq 2\Lambda$. Then

$$\left| \frac{1}{2\pi i} \int_\Gamma \zeta^{k-l-1} R(\zeta) \, d\zeta \right| \leq (2^{l+1} - 1) 2^{l+1} \Lambda^{K+1} \varrho^{-(K+1-k+l)}$$

and the term on the right hand side tends to zero as $\varrho \to \infty$. Also

$$\frac{1}{2\pi i} \int_\Gamma \zeta^{k-l-1} \prod_{r=1}^{l+1} \left(1 + \frac{\lambda_r}{\zeta} + \ldots + \frac{\lambda_r^K}{\zeta^K}\right) d\zeta$$

is equal to the coefficient of $1/\zeta$ in the expansion of the integrand, that is, to the term on the right of (2.7). The proof of the lemma is complete.

The case $l = 0$ of (2.3), for all f, follows from the definition of $f : \mathcal{S}_J \to \mathcal{S}$. Note that if $(q_k)_{k \geq 1}$ is a sequence in $C(J)$ convergent in $C(J)$ to f then, by (2.3),

$$\|f - q_k\|_{\mathcal{S}_{J'}} \to 0$$

for any closed subinterval J' of J; consequently, $Of \in C(\mathcal{S}_J, \mathcal{S})$ and $(Oq_k)_{k \geq 1}$ is convergent in $C(\mathcal{S}_J, \mathcal{S})$ to Of.

The divided difference $f^{[l]}$ is bounded by the derivative $d^l f$ ([5], p. 6) and it follows that if $f \in C^l(J)$ and equation (2.2) holds then, if $A \in \mathcal{S}_{J'}$,

$$\begin{aligned}\|d^l f(A)\| &= \sup_{\|H_1\|\le 1,\ldots,\|H_l\|\le 1} \|d^l f(A)(H_1,\ldots,H_l)\| \\ &\le \sup_{\|H_1\|\le 1,\ldots,\|H_l\|\le 1} N \sup_{1\le j_0,j_l\le N} |\langle d^l f(A)(H_1,\ldots,H_l)e_{j_l}, e_{j_0}\rangle| \le N^l l! \|d^l f\|_{J'}.\end{aligned}$$

Thus for $l \ge 1$ the inequality (2.3) is a consequence of equation (2.2) which has been shown to hold if $f = p_k$ ($k = 0, 1, \ldots$). Let $\mathcal{P}$ be the space of real polynomial functions. Then, by linearity, if $f \in \mathcal{P}$ then $f \in C^\infty(\mathcal{S}, \mathcal{S})$ and (2.2) and (2.3) hold. It follows easily from the inequality (2.3) that, for each $L \ge 1$, the mapping

$$O : \mathcal{P}\ (\subseteq C^L(\mathbb{R})) \to C^L(\mathcal{S}, \mathcal{S})$$

is continuous.

Now consider $g \in C^L(J)$ and let $(q_k)_{k\ge 1}$ be a sequence of polynomials convergent to g in the space $C^L(J)$. Then $(Oq_k)_{k\ge 1}$ is a sequence in $C^L(\mathcal{S}, \mathcal{S})$. Let J' be a closed subinterval of J. Then, for $A \in \mathcal{S}_{J'}$ and $0 \le l \le L$, by (2.3) for polynomials,

$$\|d^l(Oq_k - Oq_j)(A)\| \le N^l l! \|d^l(q_k - q_j)\|_{J'}.$$

Thus

$$\|d^l(Oq_k - Oq_j)\|_{\mathcal{S}_{J'}} \le N^l l! \|d^l(q_k - q_j)\|_{J'}.$$

The sequence $(q_k)_{k\ge 1}$ is a Cauchy sequence in $C^L(J)$ and it now follows that $(Oq_k)_{k\ge 1}$ is a Cauchy sequence in $C^L(\mathcal{S}_J, \mathcal{S})$. Let q be the limit in $C^L(\mathcal{S}_J, \mathcal{S})$ of $(Oq_k)_{k\ge 1}$. Then, for each $A \in \mathcal{S}_J$,

$$q(A) = \lim_{k\to\infty} Oq_k(A) = Og(A).$$

Therefore $Og = q \in C^L(\mathcal{S}_J, \mathcal{S})$ and $Og = \lim_{k\to\infty} Oq_k$. Furthermore, for $l = 0, \ldots, L$,

$$g^{[l]} = \lim_{k\to\infty} q_k^{[l]}.$$

The formula (2.2) holds for $f = q_k,\ k = 1, 2, \ldots,$ and it follows that it holds for $f = g$. The proof of the theorem is complete.

The matrix representation (2.2) of the first Fréchet derivative dOf of the operator function Of is well known and appears frequently in the literature. However there is an equivalent operator-theoretic form which shows that there is a sense in which, if $N \ge 2$, the derivative of the operator function Of contains both the operator function Of' and the operator function Of. Note that for $A \in \mathcal{S}$ each operator $T \in \mathcal{S}$ can be represented in the form $K + i(HA - AH)$ where $K, H \in \mathcal{S}$ and $KA = AK$; with the notation of equation (2.1) one can take

$$K = \sum_j E_j T E_j \quad \text{and} \quad H = \sum_{j\ne k} \frac{i}{\lambda_j - \lambda_k} E_j T E_k.$$

If the eigenvalues of A are distinct this decomposition of T corresponds to the decomposition of a matrix into its diagonal and off-diagonal parts.

THEOREM 2.4. *Suppose* $f \in C^1(J)$ *and* $A \in \mathcal{S}_J$. *If* $K, H \in \mathcal{S}$ *and* $KA = AK$ *then*

$$df(A)(K + i(HA - AH)) = f'(A)K + i(Hf(A) - f(A)H). \tag{2.8}$$

PROOF. For the monomials p_k $(k = 0, 1, \ldots)$ the formula (2.8) follows by direct calculation from the case $l = 1$ of 2.4, and it extends by linearity to all polynomials and then, by Theorem 2.1, by continuity to all $f \in C^1(J)$.

Using the preceding theorem it is possible to recapture the operator functions Of from their derivatives dOf algebraically.

For notational purposes regard an $h \in \mathbb{C}^N$ as a column vector. For $H \in \mathcal{S}(\mathbb{C}^N \oplus \mathbb{C})$ let $M(H)$ denote the natural (block) matrix of the operator H. Let

$$T : \mathbb{C}^N \to \mathcal{S}(\mathbb{C}^N \oplus \mathbb{C})$$

be the real linear mapping defined by

$$M(Th) = \begin{bmatrix} 0 & h \\ h^* & 0 \end{bmatrix} \tag{2.9}$$

and let

$$P : \mathcal{S}(\mathbb{C}^N \oplus \mathbb{C}) \to \mathbb{C}^N$$

be the left inverse of T defined by

$$P(H) = h \quad \text{if} \quad M(H) = \begin{bmatrix} A & h \\ h^* & \lambda \end{bmatrix}. \tag{2.10}$$

If B is an operator on a space let δ_B denote the derivation on the space of operators defined by

$$\delta_B(H) = HB - BH. \tag{2.11}$$

It follows from Theorem 2.4 that if $f \in C^1(J)$ and $A \in \mathcal{S}_J$ then

$$df(A)\delta_{iA} = \delta_{if(A)}. \tag{2.12}$$

In the following theorem we require that $0 \in J$ in order that $A \oplus 0 \in \mathcal{S}_J(\mathbb{C}^{N+1})$ whenever $A \in \mathcal{S}_J(\mathbb{C}^N)$. The identity operator on $\mathbb{C}^N$ is denoted by I.

THEOREM 2.5. *Suppose* $0 \in J$. *If* $f \in C^1(J)$ *and* $A \in \mathcal{S}_J$ *then*

$$f(A) = f(0)I - iPdf(A \oplus 0)\delta_{i(A\oplus 0)}T,$$

where T, P *and* δ *are as defined in* (2.9)–(2.11).

The proof is a simple calculation using (2.12) and the fact that $f(A\oplus 0) = f(A) \oplus f(0)$. The operators Th occur in Lemma 3.7 of [9].

3. Operator monotonicity and convexity

DEFINITIONS. A function $f : J \to \mathbb{R}$ is said to be *operator monotone* if

$$A, B \in \mathcal{S}_J,\ A \le B \ \Rightarrow\ f(A) \le f(B). \tag{3.1}$$

The condition is equivalent to the condition that, for each $N \in \mathbb{N}$, the real function $\langle f(A+tH)\xi, \xi\rangle$ of t is increasing on the set $\{t \in \mathbb{R} : A+tH \in \mathcal{S}_J\}$ for all $A \in \mathcal{S}_J, H \in \mathcal{S}$ such that $H \geq 0$ and $\xi \in \mathbb{C}^N$. In Section 4 we consider operator functions of two variables and here we define convexity in a suitably general context. Let W be a convex subset of a real linear space X. A mapping

$$F : W \to \mathcal{S}(\mathbb{C}^N)$$

will be said to be *convex* if

$$F((1-t)A+tB) \leq (1-t)F(A)+tF(B) \tag{3.2}$$

for all $A, B \in W$ and all $t \in [0,1]$. The condition (3.2) is equivalent to the condition that $\langle F(A+tH)\xi, \xi\rangle$ is a convex function of t on the convex subset $\Omega = \{t : A+tH \in W\}$ of $\mathbb{R}$ for all $A \in W, H \in X$ and $\xi \in \mathbb{C}^N$.

A function $f : J \to \mathbb{R}$ is said to be *operator convex* if each of the mappings $Of : \mathcal{S}_J(\mathbb{C}^N) \to \mathcal{S}(\mathbb{C}^N)$ $(N \in \mathbb{N})$ is convex. The function $f : J \to \mathbb{R}$ is said to be *operator concave* if $-f$ is operator convex.

There is an intimate relation between operator monotonicity and operator convexity which features prominently in [9], and operator convex functions are also analytic. It is natural to seek to apply the calculus to the consideration of operator monotonicity and operator convexity.

At several points in the discussion we will appeal to the fact that, by 3.1.4 and 3.6.1 of [6],

$$\langle d^l f(A)(H,\ldots,H)\xi, \xi\rangle = \frac{d^l}{dt^l}\langle f(A+tH)\xi, \xi\rangle\bigg|_{t=0}. \tag{3.3}$$

For sufficiently differentiable functions the elementary differential characterisations of monotonicity and convexity extend immediately to operator functions.

Theorem 3.1. *If $f \in C^1(J)$ then f is operator monotone if and only if, for each $N \in \mathbb{N}$, $df(A)(H) \geq 0$ whenever $A \in \mathcal{S}_J, H \in \mathcal{S}$ and $H \geq 0$.*

Proof. The second condition of the theorem is equivalent, by equation (3.3), to the condition that

$$\frac{d}{dt}\langle f(A+tH)\xi, \xi\rangle\bigg|_{t=0} \geq 0.$$

The latter condition is easily seen to be equivalent to the operator monotonicity of f.

For convexity it is appropriate to formulate a theorem in the general context.

Theorem 3.2. *Let W be an open convex subset of a real normed linear space X. Suppose that $F \in C^2(W, \mathcal{S}(\mathbb{C}^N))$. Then F is convex if and only if*

$$d^2F(A)(H,H) \geq 0$$

for all $A \in W$ and $H \in X$.

Proof. The second condition of the theorem is equivalent, by equation (3.3), to the condition that

$$\frac{d^2}{dt^2}\langle F(A+tH)\xi,\xi\rangle\Big|_{t=0} \geq 0.$$

for all $A \in W, H \in X$ and $\xi \in \mathbb{C}^N$. The latter condition is easily seen to be equivalent to the convexity of F.

Matrix forms of Theorem 3.1 and of Theorem 3.2 in the case of operator functions now follow immediately from equation (2.2) of Theorem 2.1. In the monograph [5], Chap.VII, Theorem 3.1 appears implicitly and its matrix form explicitly. A matrix form of Theorem 3.2 is given in [11].

In the rest of this section we are concerned with two examples: the functions $1/t$ and t^α $(\alpha > 0)$.

Proposition 3.3. *Let $p_{-1}(t) = 1/t$ for $t \in \mathbb{R} \setminus \{0\}$, and consider either $J = (-\infty, 0)$ or $J = (0,\infty)$ and $p_{-1} \in C^\infty(J)$. Then, for each $l \geq 1$,*

$$d^l p_{-1}(A)(H,\dots,H) = l!(-1)^l(A^{-1}H)^l A^{-1} \tag{3.4}$$

for each $A \in \mathcal{S}_J$ and each $H \in \mathcal{S}$.

Proof. Equation (3.4) follows from the Neumann series

$$p_{-1}(A+tH) = \sum_{l=0}^{\infty}(-1)^l t^l (A^{-1}H)^l A^{-1}$$

together with equation (3.3).

From the cases $l = 1$,

$$dp_{-1}(A)(H) = -A^{-1}HA^{-1},$$

and $l = 2$,

$$d^2p_{-1}(A)(H,H) = 2A^{-1}HA^{-1}HA^{-1} = 2(HA^{-1})^*A^{-1}(HA^{-1})$$

of (3.4) together with Theorems 3.1 and 3.2 the following well known facts follow immediately.

Corollary 3.4. *The function $-1/t$ is operator monotone on both $(-\infty, 0)$ and $(0,\infty)$, is operator convex on $(-\infty, 0)$ and operator concave on $(0,\infty)$.*

Next we consider the functions $p_\alpha \in C^\infty((0,\infty))$, for $\alpha \geq 0$, defined by

$$p_\alpha(t) = t^\alpha = \exp(\alpha \log t).$$

It follows immediately from Löwner's characterisation of operator monotone functions, by considering the analytic extension of p_α to $\mathbb{C} \setminus (-\infty, 0)$, that p_α is operator monotone on $(0,\infty)$ if and only if $0 \leq \alpha \leq 1$. The most elegant and elementary proof of this result is due to Pedersen [15]. It does not seem possible to obtain a simple direct proof of the result by considering the Fréchet derivatives of the operator functions Op_α. We obtain instead conditions which are equivalent to the operator monotonicity of p_α. Using Theorem 2.4 we obtain the following theorem.

THEOREM 3.5. *Let $\alpha > 0$. Then the following three conditions are equivalent*:

(1) $0 < \alpha \le 1$.

(2) *The function p_α is operator monotone on $(0, \infty)$.*

(3) *For each $N \in \mathbb{N}$,*

$$K + \frac{i}{\alpha}(B^{-\alpha} H B^{\alpha} - B^{\alpha} H B^{-\alpha}) \ge 0$$

whenever $B \in \mathcal{S}_{(0,\infty)}$, $K, H \in \mathcal{S}$, $KB = BK$ and

$$K + i(B^{-1} H B - B H B^{-1}) \ge 0.$$

PROOF. The equivalence of (1) and (2) is well known (see above). Let $A, B \in \mathcal{S}_{(0,\infty)}, K, H \in \mathcal{S}$ and $A = B^2, H = BH_1B$. Then

$$K + i(B^{-1} H B - B H B^{-1}) = K + i(H_1 A - A H_1)$$

and, by Theorem 2.4,

$$K + \frac{i}{\alpha}(B^{-\alpha} H B^{\alpha} - B^{\alpha} H B^{-\alpha}) = \frac{1}{\alpha} B^{1-\alpha} dp_\alpha(A)(K + i(H_1 A - A H_1)) B^{1-\alpha}.$$

The equivalence of (2) and (3) now follows from Theorem 3.1.

There is a second approach to the operator monotonicity of p_α. It is enough to consider rational α. If $m, n \in \mathbb{N}$ then $p_{m/n} = p_n^{-1} \circ p_m$.

If $f,\ g,\ h$ are real-valued functions defined on open subintervals of $\mathbb{R}$ and $f = g \circ h$ then $Of = Og \circ Oh$. If $g = h^{-1}$ then $Og = (Oh)^{-1}$. If f, g, h are continuously differentiable then so are the corresponding operator functions and $d(Of)(A) = d(Og)(h(A)) \circ d(Oh)(A)$. It follows that if $m, n \in \mathbb{N}$ then for each $A \in \mathcal{S}_{(0,\infty)}$ the derivative $dp_n(A)$ is invertible and

$$dp_{m/n}(A) = (dp_n(A^{m/n}))^{-1} \circ dp_m(A).$$

The derivatives of Op_m and Op_n are given by equation (2.4) and so using the equivalence of (1) and (2) of Theorem 3.5 together with Theorem 3.1 we obtain the following result.

THEOREM 3.6. *If $n \in \mathbb{N}$ then for each $A \in \mathcal{S}_{(0,\infty)}$ and $H \in \mathcal{S}$ the equation*

$$\sum_{r=0}^{n-1} A^r K A^{n-1-r} = H$$

has a unique solution $K \in \mathcal{S}$.

If $m, n \in \mathbb{N}$ then the following statements are equivalent:

(1) $m \le n$.

(2) *The function $p_{m/n}$ is operator monotone on $(0, \infty)$.*

(3) *If $B \in \mathcal{S}_{(0,\infty)}$ and $H, K \in \mathcal{S}$, $H \ge 0$ and*

$$\sum_{r=0}^{n-1} B^{mr} K B^{m(n-1-r)} = \sum_{r=0}^{m-1} B^{nr} H B^{n(m-1-r)}$$

then $K \ge 0$.

In the case $m = 1,\ n = 2$ the theorem is contained in a result known as *Lyapunov's theorem* (see [14] for references). If $m = 1, n = 3$ then assertion (3) is contained in results of Kwong [12].

4. Operator functions of two variables

In this section the definition of operator functions of two variables due to Korányi [10] is recalled, the analogue for two variables of Theorem 2.1 is obtained and we begin the consideration of operator convexity of functions of two variables. It is shown that the calculus provides a natural proof of a theorem, deduced by Aujla [2] from a result of Ando [1], which identifies certain operator convex functions of two variables.

Definition. Let J and J' be open subintervals of $\mathbb{R}$ and let $M, N \in \mathbb{N}$. For a function $f : J \times J' \to \mathbb{R}$ there is an associated operator function

$$f = Of : \mathcal{S}_J(\mathbb{C}^M) \times \mathcal{S}_{J'}(\mathbb{C}^N) \to \mathcal{S}(\mathbb{C}^M \otimes \mathbb{C}^N)$$

defined in the following way. If $(A, B) \in \mathcal{S}_J(\mathbb{C}^M) \times \mathcal{S}_{J'}(\mathbb{C}^N)$ and

$$A = \sum_j \lambda_j E_j, \qquad B = \sum_k \mu_k F_k$$

are the spectral resolutions of A and B respectively then

$$f(A, B) = \sum_j \sum_k f(\lambda_j, \mu_k) E_j \otimes F_k.$$

The tensor product $\mathbb{C}^M \otimes \mathbb{C}^N$ has inner product defined by

$$\langle a \otimes b, a' \otimes b' \rangle = \langle a, a' \rangle \langle b, b' \rangle.$$

For the purposes of our calculations the space $\mathcal{S}(\mathbb{C}^M) \times \mathcal{S}(\mathbb{C}^N)$ will be normed by

$$\|(H, K)\| = \max\{\|H\|, \|K\|\}. \tag{4.1}$$

The main result of this section is a two-variable analogue of Theorem 2.1 concerning functions $f \in C^L(J \times J')$, the space of L times continuously Fréchet differentiable functions defined on the open subset $J \times J'$ of $\mathbb{R}^2$. If $f \in C^L(J \times J')$ and $l + m \le L$ let $f^{(l,m)}$ denote the (equal) partial derivatives of f in which f is differentiated l times with respect to the first variable and m times with respect to the second variable. For such a function f we will denote by

$$f^{[l,m]}(\lambda_1, \dots, \lambda_{l+1}; \mu_1, \dots, \mu_{m+1})$$

the repeated divided difference of f, with respect to the first variable on the points $\lambda_1, \dots, \lambda_{l+1}$ in J and then with respect to the second variable on the points $\mu_1, \dots, \mu_{m+1}$ in J'. The following lemma is required.

Lemma 4.1. *Suppose $f \in C^L(J \times J')$ and $l + m \le L$. If J_1, J_1' are closed subintervals of J and J' respectively, and $\lambda_1, \dots, \lambda_{l+1} \in J_1$, $\mu_1, \dots, \mu_{m+1} \in J_1'$ then, for some $(\xi, \zeta) \in J_1 \times J_1'$,*

$$f^{[l,m]}(\lambda_1, \dots, \lambda_{l+1}; \mu_1, \dots, \mu_{m+1}) = \frac{1}{l!m!} f^{(l,m)}(\xi, \zeta).$$

Proof. The proof is by deduction from the one-variable result. By the Lemma of [5],

p. 6, there exist $\zeta \in J_1'$ and $\xi \in J_1$ such that

$$\begin{aligned} f^{[l,m]}(\lambda_1,\ldots,\lambda_{l+1};\mu_1,\ldots,\mu_{m+1}) &= f^{[l,0]}(\lambda_1,\ldots,\lambda_{l+1};\mu)^{[m]}(\mu_1,\ldots,\mu_{m+1}) \\ &= \frac{1}{m!}\frac{\partial^m}{\partial\mu^m} f^{[l,0]}(\lambda_1,\ldots,\lambda_{l+1};\mu)\bigg|_{\mu=\zeta} \\ &= \frac{1}{m!}\left(\frac{\partial^m f}{\partial\mu^m}\bigg|_{\mu=\zeta}\right)^{[l]}(\lambda_1,\ldots,\lambda_{l+1}) \\ &= \frac{1}{m!}\frac{1}{l!}\frac{\partial^l}{\partial\lambda^l}\left(\frac{\partial^m f}{\partial\mu^m}\bigg|_{\mu=\zeta}\right)\bigg|_{\lambda=\xi} \\ &= \frac{1}{m!}\frac{1}{l!} f^{(l,m)}(\xi,\zeta) \end{aligned}$$

(where the central equality expresses the fact that the divided difference operator in the first variable commutes with the partial differential operator in the second variable).

It follows immediately from the definition of the operator function that if $f(s,t) = g(s)h(t)$ for $(s,t) \in J\times J'$ then $f(A,B) = g(A)\otimes h(B)$ for all $(A,B) \in \mathcal{S}_J(\mathbb{C}^M)\times\mathcal{S}_{J'}(\mathbb{C}^N)$. It is easily seen that for such a function $f \in C^L(J\times J')$, if $l+m \le L$ then

$$f^{[l,m]}(\lambda_1,\ldots,\lambda_{l+1};\mu_1,\ldots,\mu_{m+1}) = g^{[l]}(\lambda_1,\ldots,\lambda_{l+1})h^{[m]}(\mu_1,\ldots,\mu_{m+1}). \tag{4.2}$$

Theorem 4.2. *If $f \in C^L(J\times J')$ then*

$$Of \in C^L(\mathcal{S}_J(\mathbb{C}^M)\times\mathcal{S}_{J'}(\mathbb{C}^N), \mathcal{S}(\mathbb{C}^M\otimes\mathbb{C}^N)).$$

The mapping

$$O : C^L(J\times J') \to C^L(\mathcal{S}_J(\mathbb{C}^M)\times\mathcal{S}_{J'}(\mathbb{C}^N), \mathcal{S}(\mathbb{C}^M\otimes\mathbb{C}^N))$$

is continuous.

If $f \in C^L(J\times J')$ and J_1 and J_1' are closed subintervals of J and J' respectively then for $0 \le l \le L$,

$$\|d^l f\|_{\mathcal{S}_{J_1}\times\mathcal{S}_{J_1'}} \le \sum_{r=0}^{l} c_{l,r}(M,N)\|f^{(r,l-r)}\|_{J_1\times J_1'}, \tag{4.3}$$

for some coefficients $c_{l,r}(M,N)$.

Proof. The pattern of proof is similar to that of Theorem 2.1 but begins with the consideration of functions of the form $f(s,t) = g(s)h(t)$. For these functions there is a straightforward lemma.

Lemma 4.3. *Suppose that $g \in C^L(J)$, $h \in C^L(J')$ and that $f(s,t) = g(s)h(t)$ for all $(s,t) \in J\times J'$. Then $Of \in C^L(\mathcal{S}_J(\mathbb{C}^M)\times\mathcal{S}_{J'}(\mathbb{C}^N), \mathcal{S}(\mathbb{C}^M\otimes\mathbb{C}^N))$ and, for $1 \le l \le L$,*

$$\begin{aligned} &d^l f(A,B)((H_1,K_1),\ldots,(H_l,K_l)) \\ &\quad = \sum_{r=0}^{l}\sum_{\sigma\in S_l}\frac{1}{r!(l-r)!} d^r g(A)(H_{\sigma(1)},\ldots,H_{\sigma(r)})\otimes d^{l-r}h(B)(K_{\sigma(r+1)},\ldots,K_{\sigma(l)}). \end{aligned}$$

The proof of the lemma is a technical exercise and is omitted.

The case $l = 0$ of the inequality (4.3) follows, for all f, from the definition of the operator function. Now suppose that f is as in the lemma. If $A \in \mathcal{S}_J(\mathbb{C}^M)$ and $B \in$

$\mathcal{S}_{J'}(\mathbb{C}^N)$ let $a_1,\dots,a_M$ be an orthonormal basis of $\mathbb{C}^M$ consisting of eigenvectors of A corresponding to eigenvalues $\lambda_1,\dots,\lambda_M$ and let $b_1,\dots,b_N$ be an orthonormal basis of $\mathbb{C}^N$ consisting of eigenvectors of B corresponding to eigenvalues $\mu_1,\dots,\mu_N$. Then $a_j\otimes b_k$, $j=1,\dots,M$, $k=1,\dots,N$, is an orthonormal basis of $\mathbb{C}^M\otimes\mathbb{C}^N$. For $1\le l\le L$ we obtain the matrix of $d^l(A,B)((H_1,K_1)\dots,(H_l,K_l))$ with respect to this basis from the equation of Lemma 4.3, equation (2.2) applied to each of the terms of that equation involving g and h, the definition of $g(A)$ and $h(B)$, and equation (4.2):

$$\tag{4.4} \begin{aligned}&\langle d^l f(A,B)((H_1,K_1),\dots,(H_l,K_l))a_j\otimes b_k, a_{j'}\otimes b_{k'}\rangle\\ &\qquad = \sum_{r=0}^{l}\sum_{\sigma\in S_l}\frac{1}{r!(l-r)!}\sum_{1\le j_1,\dots,j_{r-1}\le M}\;\sum_{1\le k_1,\dots,k_{l-r-1}\le N} F\times C,\end{aligned}$$

where, if $r\ge 2$ and $l-r\ge 2$,

$$F = f^{[r,l-r]}(\lambda_{j'},\lambda_{j_1},\dots,\lambda_{j_{r-1}},\lambda_j;\mu_{k'},\mu_{k_1},\dots,\mu_{k_{l-r-1}},\mu_k)$$

and

$$\begin{aligned}C = &\Big(\sum_{\nu\in S_r}\langle H_{\sigma(\nu(1))}a_{j_1},a_{j'}\rangle\prod_{s=2}^{r-1}\langle H_{\sigma(\nu(s))}a_{j_s},a_{j_{s-1}}\rangle\langle H_{\sigma(\nu(r))}a_j,a_{j_{r-1}}\rangle\Big)\\ &\times\Big(\sum_{\tau\in S_{l-r}}\langle K_{\sigma(r+\tau(1))}b_{k_1},b_{k'}\rangle\prod_{t=2}^{l-r-1}\langle K_{\sigma(r+\tau(t))}b_{k_t},b_{k_{t-1}}\rangle\langle K_{\sigma(r+\tau(l-r))}b_k,b_{k_{l-r-1}}\rangle\Big).\end{aligned}$$

The factors F and C are of a similar form in the other cases. Formula (4.4) extends by linearity to the set $\mathcal{F}$ of all functions $f\in C^L(J\times J')$ which are finite sums of products of functions of one variable. In the "general" case the coefficient C is a sum of $r!(l-r)!$ products each of $l=r+(l-r)$ terms. Each product involves just one of each of the pairs $(H_1,K_1),\dots,(H_l,K_l)$. Now, using Lemma 4.1 and the norm (4.1), it follows that, for $(A,B)\in\mathcal{S}_{J_1}(\mathbb{C}^M)\times\mathcal{S}_{J_1'}(\mathbb{C}^N)$,

$$\begin{aligned}&|\langle d^l f(A,B)((H_1,K_1),\dots,(H_l,K_l))a_j\otimes b_k,a_{j'}\otimes b_{k'}\rangle|\\ &\qquad\le\sum_{r=0}^{l}c'_{l,r}(M,N)\|f^{(r,l-r)}\|_{I'\times J'}\prod_{m=1}^{l}\|(H_m,K_m)\|\end{aligned}$$

for certain coefficients $c'_{l,r}(M,N)$. The inequality (4.3) for $f\in\mathcal{F}$ now follows, with $c=MNc'$. This proves that the mapping of $\mathcal{F}$ into $C^L(\mathcal{S}_J(\mathbb{C}^M)\times\mathcal{S}_{J'}(\mathbb{C}^N),\mathcal{S}(\mathbb{C}^M\otimes\mathbb{C}^N))$ is continuous. The proof of Theorem 4.2 is now completed in the same way as was the proof of Theorem 2.1 using the fact that $\mathcal{F}$ is dense in the space $C^L(J\times J')$.

It is an open problem to determine which functions $f: J\times J'\to\mathbb{R}$ are operator convex. An operator convex function of two variables is necessarily operator convex in each variable separately and is itself convex on $J\times J'$ (the case $M=N=1$). However, the verification that a function of two variables is operator convex may not be easy. The following interesting theorem was deduced, in a slightly more restricted form, by Aujla [2] from a more limited result obtained by Ando [1]. It will be shown that the calculus provides a natural and straightforward proof of the theorem, quite different from the original proof.

THEOREM 4.4. *Suppose that $g \in C^2(J)$, $h \in C^2(J')$ and that g and h are both positive and operator concave. Then the function*

$$f(s,t) = \frac{1}{g(s)h(t)}$$

is an operator convex function of two variables on $J \times J'$.

The proof of the theorem requires the following lemma.

LEMMA 4.5. *If $g \in C^2(J)$, g is positive and $\mathbf{G}(s) = 1/g(s) = (p_{-1} \circ g)(s)$ then, for all $A \in \mathcal{S}_J(\mathbb{C}^M)$ and all $H \in \mathcal{S}(\mathbb{C}^M)$,*

$$d\mathbf{G}(A)(H) = -g(A)^{-1}dg(A)(H)g(A)^{-1} \tag{4.5}$$

and

$$d^2\mathbf{G}(A)(H,H) = g(A)^{-1}(-d^2g(A)(H,H) + 2dg(A)(H)g(A)^{-1}dg(A)(H))g(A)^{-1}. \tag{4.6}$$

PROOF. The operator O respects composition of functions: $O\mathbf{G} = Op_{-1} \circ Og$. Equation (4.5) is given by the chain rule for partial derivatives together with equation (3.4). The proof of equation (4.6) is a more involved technical exercise which we omit.

PROOF OF THEOREM 4.4. Suppose that f, g and h are as in the statement of the theorem. Let

$$\mathbf{G}(s) = \frac{1}{g(s)}, \quad \mathbf{H}(t) = \frac{1}{h(t)},$$

so that

$$f(s,t) = \mathbf{G}(s)\mathbf{H}(t).$$

Then by Theorem 3.2 and Lemma 4.1 the function f is operator convex on $J \times J'$ if and only if for each $M, N \in \mathbb{N}$ and for all $A \in \mathcal{S}_J(\mathbb{C}^M)$, $B \in \mathcal{S}_{J'}(\mathbb{C}^N)$, $H \in \mathcal{S}(\mathbb{C}^M)$ and $K \in \mathcal{S}(\mathbb{C}^N)$,

$$\begin{aligned} 0 &\le d^2f(A,B)((H,K),(H,K)) \\ &= \mathbf{G}(A) \otimes d^2\mathbf{H}(B)(K,K) + 2d\mathbf{G}(A)(H) \otimes d\mathbf{H}(B)(K) \\ &\quad + d^2\mathbf{G}(A)(H,H) \otimes \mathbf{H}(B). \end{aligned} \tag{4.7}$$

By Lemma 4.5,

$$\begin{aligned} &(g(A) \otimes h(B))d^2f(A,B)((H,K),(H,K))(g(A) \otimes h(B)) \\ &\qquad = g(A) \otimes (-d^2h(B)(K,K) + 2dh(B)(K)h(B)^{-1}dh(B)(K)) \\ &\qquad\quad + 2dg(A)(H) \otimes dh(B)(K) \\ &\qquad\quad + (-d^2g(A)(H,H) + 2dg(A)(H)g(A)^{-1}dg(A)(H)) \otimes h(B). \end{aligned} \tag{4.8}$$

By the positivity of g and h, condition (4.7) is equivalent to the condition that the operator (4.8) is non-negative. By the positivity and operator concavity of g and h the first and fourth of the five summands in (4.8) are non-negative. However, the sum of the remaining terms is

$$\begin{aligned}
&g(A)\otimes dh(B)(K)h(B)^{-1}dh(B)(K)\\
&\quad + dg(A)(H)\otimes dh(B)(K) + dg(A)(H)g(A)^{-1}dg(A)(H)\otimes h(B)\\
&= I\otimes dh(B)(K)\, g(A)\otimes h(B)^{-1}\, I\otimes dh(B)(K) + I\otimes dh(B)(K)\, dg(A)(H)\otimes I\\
&\quad + dg(A)(H)\otimes I\, g(A)^{-1}\otimes h(B)\, dg(A)(H)\otimes I\\
&= \left[I\otimes dh(B)(K)\, g(A)^{1/2}\otimes h(B)^{-1/2} + \frac{1}{2}dg(A)(H)\otimes I\, g(A)^{-1/2}\otimes h(B)^{1/2}\right]\\
&\quad \times\left[g(A)^{1/2}\otimes h(B)^{-1/2}\, I\otimes dh(B)(K) + \frac{1}{2}g(A)^{-1/2}\otimes h(B)^{1/2}\, dg(A)(H)\otimes I\right]\\
&\quad + \frac{3}{4}dg(A)(H)\otimes I g(A)^{-1}\otimes h(B)\, dg(A)(H)\otimes I.
\end{aligned}$$

The first term in the latter sum is the product of an operator and its adjoint and so is non-negative; the second term is non-negative because g and h are non-negative and $dg(A)(H)\otimes I$ is self-adjoint. The proof of the theorem is complete.

COROLLARY 4.6. *If* $(\alpha,\beta)\in[-1,1]^2$ *then the function*

$$f(s,t)=\frac{1}{(1-\alpha s)(1-\beta t)}$$

is an operator convex function on $(-1,1)\times(-1,1)$.

Hansen [7] has extended the result of the corollary to any number of variables with a different proof. The result of the corollary, and the extension, can be proved by a straightforward calculation of the second Fréchet derivative and application of Thm. 3.2 in the following way.

Suppose $\alpha_1,\ldots,\alpha_k\in[0,1]$ and that for $j=1,\ldots,k$ the function $f_j:(-1,1)\to\mathbb{R}$ is defined by $f_j(t)=(1-\alpha_j t)^{-1}$. Let $f:(-1,1)^k\to\mathbb{R}$ be defined by

$$f(t_1,\ldots,t_k)=\prod_{j=1}^{k} f_j(t_j).$$

Then the operator function

$$\mathcal{O}f:\prod_{j=1}^{k}\mathcal{S}_{(-1,1)}(\mathbb{C}^{N_j})\to\bigotimes_{j=1}^{k}\mathcal{S}(\mathbb{C}^{N_j})$$

is given by

$$\mathcal{O}f(A_1,\ldots,A_k)=\bigotimes_{j=1}^{k}\mathcal{O}f_j(A_j).$$

The operator functions $\mathcal{O}f_j$ are infinitely Fréchet differentiable and it follows that $\mathcal{O}f$ is infinitely differentiable. Now put $B_j=(I-\alpha_j A_j)^{-1/2},\ K_j=B_jH_jB_j$ and

$$K_j'=I\otimes\ldots\otimes I\otimes K_j\otimes I\otimes\ldots\otimes I$$

for $j = 1, \ldots, k$. Then, for small $H_1, \ldots, H_k$,

$$f(A_1 + H_1, \ldots, A_k + H_k) = \bigotimes_{j=1}^{k} B_j^2 \sum_{r=0}^{\infty} \Big(\alpha_j H_j B_j^2\Big)^r$$
$$= \Big(\bigotimes_{j=1}^{k} B_j\Big)\Big(\bigotimes_{j=1}^{k} \sum_{r=0}^{\infty} (\alpha_j K_j)^r\Big)\Big(\bigotimes_{j=1}^{k} B_j\Big).$$

The second derivative of the operator function f is given by the terms which are of degree two in $H_1, \ldots, H_k$ in the expansion of the inner tensor product; that is,

$$D^2 f(A_1, \ldots, A_k)(H_1, \ldots, H_k)^2 = 2\Big(\bigotimes_{j=1}^{k} B_j\Big)\Big(\sum_{1 \le i < j \le k} \alpha_i \alpha_j K_i' K_j' + \sum_{j=1}^{k} \alpha_j^2 K_j'^2\Big)\Big(\bigotimes_{j=1}^{k} B_j\Big)$$
$$= \Big(\bigotimes_{j=1}^{k} B_j\Big)\Big(\Big(\sum_{j=1}^{k} \alpha_j K_j'\Big)^2 + \sum_{j=1}^{k} \alpha_j^2 K_j'^2\Big)\Big(\bigotimes_{j=1}^{k} B_j\Big) \ge 0,$$

from which it follows that f is operator convex.

II. OPERATOR CONVEX FUNCTIONS OF TWO VARIABLES

5. Preliminaries

First we must present that information about operator convex functions of one variable which is necessary to the subsequent discussion.

Let $\mathcal{OC}_1$ denote the set of operator convex functions $f : (-1,1) \to \mathbb{R}$, and let $\mathcal{L}_1$ denote the set of linear functions on $(-1,1)$, i.e. functions of the form

$$l(t) = a + bt \quad \text{for all } t \in (-1,1)$$

where $a, b \in \mathbb{R}$. Thus $\mathcal{OC}_1$ is a convex cone and $\mathcal{L}_1 \subseteq \mathcal{OC}_1$. Operator convex functions of one variable are described by the following representation theorem.

THEOREM 5.1 (see [3] and [9], Thm. 4.5). *If $f \in \mathcal{OC}_1$ then f is analytic on $(-1,1)$. If $f \notin \mathcal{L}_1$ then there is a unique probability measure M on $[-1,1]$ such that*

$$f(t) = f(0) + f'(0)t + \frac{1}{2} f''(0) \int \frac{t^2}{1 - \alpha t}\, dM(\alpha)$$

for all $t \in (-1,1)$.

Let $\mathcal{K}_1 = \{f \in \mathcal{OC}_1 : f(0) = f'(0) = 0,\ f''(0) = 2\}$. Let $\mathbf{P}$ be the set of probability measures on $[-1,1]$, and regard $\mathbf{P}$ as a subset of the space $C([-1,1])^*$, equipped with the weak* topology. Then $\mathbf{P}$ is a compact convex set and its set of extreme points is the set $\{\delta_\alpha : \alpha \in [-1,1]\}$ of atoms of measure one. If $T : \mathbf{P} \to \mathcal{K}_1$ is the mapping defined by

$$(T\mu)(t) = \int \frac{t^2}{1 - \alpha t}\, dM(\alpha),$$

for $t \in (-1,1)$, then T is continuous with respect to the topology of pointwise convergence on $\mathcal{K}_1$ and, by the theorem, it is bijective. So the following proposition is a consequence of the theorem (although in the development of [9] facts closely related to those of the proposition are preliminaries to the theorem rather than consequences of it).

PROPOSITION 5.2. *The set $\mathcal{K}_1$ is convex, compact in the topology of pointwise convergence, and its set of extreme points is the set of functions of the form $t^2(1-\alpha t)^{-1}$ with $\alpha \in [-1,1]$.*

It follows from the theorem that $\mathcal{OC}_1 = \mathcal{L}_1 + \mathbb{R}^+\mathcal{K}_1$, and that the representation of $f \in \mathcal{OC}_1$ as $f = l + k$ where $l \in \mathcal{L}_1$ and $k \in \mathbb{R}^+\mathcal{K}_1$ is unique.

The two-dimensional space $\mathcal{L}_1$ is a (trivial) *face* (closed convex extremal non-empty subset) of the convex cone $\mathcal{OC}_1$, and any face of $\mathcal{OC}_1$ contains $\mathcal{L}_1$. If F is a non-trivial face of $\mathcal{OC}_1$, that is, $F \neq \mathcal{L}_1$, then $F \cap \mathcal{K}_1$ is a face of $\mathcal{K}_1$; and this correspondence is a bijection between the non-trivial faces of $\mathcal{OC}_1$ and the faces of $\mathcal{K}_1$. If G is a face of $\mathcal{K}_1$ then $\mathcal{L}_1 + \mathbb{R}^+G$ is the corresponding face of $\mathcal{OC}_1$. For a function $f \in \mathcal{OC}_1 \setminus \mathcal{L}_1$ it will be convenient to say that f is an *extremal function* of $\mathcal{OC}_1$ if $\mathcal{L}_1 + \mathbb{R}^+ f$ is a face of $\mathcal{OC}_1$, or if, equivalently, the function

$$\frac{2}{f''(0)}(f(t) - f(0) - f'(0)t)$$

is an extreme point of $\mathcal{K}_1$.

As an example with which we shall be concerned, note that if $\alpha \in [-1,1]$ then the function $t^2(1-\alpha t)^{-1}$ is an extreme point of $\mathcal{K}_1$ and if $\alpha \neq 0$ then $(1-\alpha t)^{-1} = 1 + \alpha t + \alpha^2 t^2 (1-\alpha t)^{-1}$ is an extremal function of $\mathcal{OC}_1$.

Theorem 5.1 characterises completely operator convex functions on $(-1,1)$. The results which follow are a contribution towards solving the corresponding problem for operator convex functions of two variables. First an appropriate notation is introduced.

If a function $f : (-1,1)^2 \to \mathbb{R}$ is an operator convex function of two variables then for each s and each t in $(-1,1)$ the functions $f(s,\cdot)$ and $f(\cdot,t)$ are operator convex functions of one variable and so are analytic on $(-1,1)$; that is, f is separately analytic in each variable. Let $\mathcal{OC}_2$ be the set of operator convex functions $f : (-1,1)^2 \to \mathbb{R}$. Let $\mathcal{K}_2$ be the set of f in $\mathcal{OC}_2$ such that

$$f(0,0) = f^{(1,0)}(0,0) = f^{(0,1)}(0,0) = 0, \quad f^{(2,0)}(0,0) + f^{(0,2)}(0,0) = 2.$$

Let $\mathcal{L}_2$ be the set of linear functions $l : (-1,1)^2 \to \mathbb{R}$, that is, functions of the form

$$l(s,t) = a + bs + ct \quad \text{for all } (s,t) \in (-1,1)^2,$$

where $a, b, c \in \mathbb{R}$.

PROPOSITION 5.3. *If $f \in \mathcal{OC}_2$, (s_0,t_0) and (s_1,t_1) are points of $(-1,1)^2$ and $f^{(2,0)}(s_0,t_0) = f^{(0,2)}(s_1,t_1) = 0$ then $f \in \mathcal{L}_2$. Consequently,*

$$\mathcal{OC}_2 = \mathcal{L}_2 + \mathbb{R}^+\mathcal{K}_2$$

and the representation of $f \in \mathcal{OC}_2$ as $f = l + k$, where $l \in \mathcal{L}_2$ and $k \in \mathbb{R}^+\mathcal{K}_2$, is unique.

PROOF. Suppose $f \in \mathcal{OC}_2$ and $f^{(2,0)}(s_0,t_0) = f^{(0,2)}(s_1,t_1) = 0$. Then, by Thm. 5.1, the functions $f(s_1,\cdot)$ and $f(\cdot,t_0)$ are linear and the graph of f contains line segments above $\{s_1\} \times (-1,1)$ and $(-1,1) \times \{t_0\}$. Therefore the support plane Π to the graph of f through the point $(s_1, t_0, f(s_1,t_0))$ is unique and contains the two line segments. The graph of f lies above Π but, by the convexity of f, that part of the graph which is above the convex hull of $(\{s_1\} \times (-1,1)) \cup ((-1,1) \times \{t_0\})$ lies beneath Π, and so in Π. Thus the restriction of f to the open quadrilateral $\operatorname{co}((\{s_1\} \times (-1,1)) \cup ((-1,1) \times \{t_0\}))$ is linear. It follows by the separate analyticity of f that it is linear on $(-1,1)^2$. This proves the first assertion of the proposition, and the second is a straightforward consequence.

The three-dimensional space $\mathcal{L}_2$ is a face of the convex cone $\mathcal{OC}_2$, any face of the cone contains $\mathcal{L}_2$. There is a bijection between the faces of $\mathcal{K}_2$ and the non-trivial faces of $\mathcal{OC}_2$. An extreme point of $\mathcal{K}_2$ corresponds to a four-dimensional face of $\mathcal{OC}_2$. A function $f \in \mathcal{OC}_2 \setminus \mathcal{L}_2$ will be said to be an *extremal function* of $\mathcal{OC}_2$ if $\mathcal{L}_2 + \mathbb{R}^+ f$ is a face of $\mathcal{OC}_2$; thus an extremal function of $\mathcal{OC}_2$ determines an extreme point of $\mathcal{K}_2$.

Suppose that $\alpha, \beta \in [-1,1]$. Then the functions $(1-\alpha s)^{-1}$ and $(1-\beta t)^{-1}$ are extremal functions of $\mathcal{OC}_1$. The function $(1-\alpha s)^{-1}(1-\beta t)^{-1}$ is in $\mathcal{OC}_2$ by Cor. 4.6 and one can describe it as being *separately extremal*. It is natural to ask whether it is extremal in $\mathcal{OC}_2$. The results in the rest of this paper flow from this question, the answer to which is “no” if $\alpha\beta \neq 0$ (Thm. 8.3(3)).

Consider, more generally, a function $f \in \mathcal{OC}_2$ which is such that for each $s \in (-1,1)$ the function $f(s,\cdot)$ is extremal in $\mathcal{OC}_1$, and for each $t \in (-1,1)$ the function $f(\cdot,t)$ is extremal in $\mathcal{OC}_1$. Then f can be represented in each of the two forms

$$f(s,t) = \lambda(s) + \mu(s)t + \nu(s)\frac{t^2}{1-\beta(s)t} \tag{5.1}$$

and

$$f(s,t) = l(t) + m(t)s + n(t)\frac{s^2}{1-\alpha(t)s}. \tag{5.2}$$

It should be noted that if $f : (-1,1)^2 \to \mathbb{R}$ is separately operator convex in each variable then it has representations

$$f(s,t) = \lambda(s) + \mu(s)t + \nu(s)\int \frac{t^2}{1-\beta t}\, dM_s(\beta) \tag{5.3}$$

and

$$f(s,t) = l(t) + m(t)s + n(t)\int \frac{s^2}{1-\alpha s}\, dN_t(\alpha). \tag{5.4}$$

The representations (5.1) and (5.2) are the special cases of the representations (5.3) and (5.4) in which the measures M_s and N_t are atoms.

The next section is devoted to the solution of the pair of equations (5.1) and (5.2) under the assumption that the functions $\alpha(t)$ and $\beta(s)$ have continuous second derivatives.

6. Separately extremal functions of two variables

We will consider the following pair of equations of which equations (5.1) and (5.2) are a particular case:

$$f(s,t) = \lambda(s) + \mu(s)t + \nu(s)t^2 k_s(t) \tag{6.1}$$

and

$$f(s,t) = l(t) + m(t)s + n(t)s^2 h_t(s) \tag{6.2}$$

where $h_t(s)$ and $k_s(t)$ are defined for $(s,t) \in (-1,1)^2$.

ASSUMPTIONS. It will be assumed that the functions $h_t(s)$ and $k_s(t)$ satisfy the following conditions:

(C0) $h_t(s)$ is separately continuous in s and t. Here and in the next three conditions it is to be understood the the corresponding condition for k obtained by replacing h by k and interchanging s and t is included.
(C1) $\frac{\partial}{\partial t} h_t(s)$ exists and is separately continuous in s and t.
(C2) $\frac{\partial^2}{\partial t^2} h_t(s)$ exists and is separately continuous in s and t,
$\frac{\partial^2}{\partial s^2} h_t(s)$ exists and is a continuous function of s, and
$\frac{\partial^2}{\partial s \partial t} h_t(s)\big|_{(0,0)}$ exists.
(C3) $\frac{\partial^2}{\partial s^2}\big(\frac{\partial}{\partial t} h_t(s)\big)\big|_{t=0}$ exists and is a continuous function of s.
(C4) $h_t(s) \neq 0$ and $k_s(t) \neq 0$ for all $(s,t) \in (-1,1)^2$.

In the present context the following condition is a convenient normalisation which lightens the calculations a little:

(C5) $h_t(0) = 1$ for all $t \in (-1,1)$, $k_s(0) = 1$ for all $s \in (-1,1)$.

For notational convenience we write

$$H_1(s) = \frac{\partial}{\partial t} h_t(s)\bigg|_{t=0}, \qquad H_2(s) = \frac{\partial^2}{\partial t^2} h_t(s)|_{t=0},$$
$$\Phi_1(t,s) = \frac{1}{t}(h_t(s) - h_0(s)), \quad \Phi_2(t,s) = \frac{1}{t^2}\bigg(h_t(s) - h_0(s) - \bigg(\frac{\partial}{\partial t} h_t(s)\bigg|_{t=0}\bigg)t\bigg).$$

The corresponding functions defined in terms of $k_s(t)$ will be denoted by $K_1(t), K_2(t)$, $\Psi_1(s,t)$ and $\Psi_2(s,t)$.

THEOREM 6.1. *Suppose that $h_t(s)$ and $k_s(t)$ are functions which satisfy conditions* (C0)–(C5). *Then a function $f : (-1,1)^2 \to \mathbb{R}$ can be represented both in the form* (6.1) *and in the form* (6.2) *for some functions λ, μ, ν, l, m, and n if and only if there are constants A, B, C, Δ, Γ_0, Γ_1, Σ_0, Σ_1 and G such that*

$$\begin{aligned} f(s,t) = {} & A + Bs + Ct + \Delta st \\ & + \Sigma_0\big(h_0(s) + H_1(s)t + \tfrac{1}{2}k_s(t)H_2(s)t^2\big)s^2 + \Sigma_1(h_0(s) + k_s(t)H_1(s)t)s^2 t \\ & + \Gamma_0 t^2 k_s(t) + \Gamma_1 s t^2 k_s(t) + \tfrac{1}{2}G k_s(t) h_0(s) s^2 t^2 \end{aligned} \tag{6.3}$$

and

$$\begin{aligned} & \Gamma_0\big(\Psi_2(s,t) - \tfrac{1}{2}h_t(s)K_2(t)\big) + \Gamma_1(\Psi_1(s,t) - h_t(s)K_1(t)) + \tfrac{1}{2}G k_s(t) h_0(s) \\ & \quad = \Sigma_0(\Phi_2(t,s) - \tfrac{1}{2}k_s(t)H_2(s)) + \Sigma_1(\Phi_1(t,s) - k_s(t)H_1(s)) + \tfrac{1}{2}G h_t(s) k_0(t), \end{aligned} \tag{6.4}$$

for all $(s,t) \in (-1,1)^2$.

PROOF. Suppose that f is both of the form (6.1) and of the form (6.2). It will be shown that $\mu'(0), m'(0), \nu''(0)$ and $n''(0)$ exist and that the relations (6.3) and (6.4) are satisfied by

$$(6.5)\qquad \begin{gathered} A=\lambda(0)=l(0), \quad B=m(0), \quad C=\mu(0), \quad \Delta=\mu'(0)=m'(0), \\ \Gamma_0=\nu(0), \quad \Gamma_1=\nu'(0), \quad \Sigma_0=n(0), \quad \Sigma_1=n'(0), \quad G=\nu''(0)=n''(0). \end{gathered}$$

It follows from (6.1) and (6.2) together with (C2) that

(C6) $\frac{\partial^2}{\partial s^2}f$ exists and is a continuous function of s, and $\frac{\partial^2}{\partial t^2}f$ exists and is a continuous function of t.

Letting $s=0$ and $t=0$ in turn we deduce that

$$(6.6)\qquad l(t)=f(0,t)=\lambda(0)+\mu(0)t+\nu(0)t^2k_0(t),$$

$$(6.7)\qquad \lambda(s)=f(s,0)=l(0)+m(0)s+n(0)s^2h_0(s).$$

Thus, by (C2),

(C7) λ'' and l'' exist and are continuous.

Substitution for l and λ, given by (6.6) and (6.7), in (6.1) and (6.2) gives

$$(6.8)\qquad f(s,t)=l(0)+m(0)s+n(0)s^2h_0(s)+\mu(s)t+\nu(s)t^2k_s(t),$$

$$(6.9)\qquad f(s,t)=\lambda(0)+\mu(0)t+\nu(0)t^2k_0(t)+m(t)s+n(t)s^2h_t(s).$$

The equality of the right hand sides of (6.8) and (6.9) leads to the equations

$$\begin{aligned} &\mu(s)-\mu(0)+(\nu(s)k_s(t)-\nu(0)k_0(t))t \\ &\qquad=\frac{m(t)-m(0)}{t}s+\frac{n(t)h_t(s)-n(0)h_0(s)}{t}s^2 \\ &\qquad=\frac{m(t)-m(0)}{t}s+\frac{n(t)-n(0)}{t}h_t(s)s^2+n(0)\frac{h_t(s)-h_0(s)}{t}s^2. \end{aligned}$$

By (C0), for each s the left hand side is convergent to $\mu(s)-\mu(0)$ as $t\to 0$, and, by (C1), the third term in the final sum is convergent to $n(0)\frac{\partial}{\partial t}h_t(s)\big|_{t=0}s^2$ as $t\to 0$. It follows that $m'(0)$ and $n'(0)$ exist and that

$$(6.10)\qquad \mu(s)=\mu(0)+m'(0)s+\frac{\partial}{\partial t}(n(t)h_t(s))\bigg|_{t=0}s^2.$$

In the same way we obtain

$$(6.11)\qquad m(t)=m(0)+\mu'(0)t+\frac{\partial}{\partial s}(\nu(s)k_s(t))\bigg|_{s=0}t^2.$$

It now follows from either (6.10) or (6.11) that $\mu'(0)=m'(0)$. It also follows, by (C2) and (C3), that

(C8) μ'' and m'' exist and are continuous.

Now, by (6.1) and (C4)

$$\nu(s)=\frac{f(s,t)-\lambda(s)-\mu(s)t}{t^2k_s(t)}$$

and so, by (C6)–(C8) and (C2), and by the corresponding argument for n,

(C9) ν'' and n'' exist and are continuous.

Substitution for μ, given by (6.10), in (6.8) gives

$$f(s,t) = l(0) + m(0)s + \mu(0)t + m'(0)st + n(0)h_0(s)s^2 + \nu(0)k_0(t)t^2 + \frac{\partial}{\partial t}(n(t)h_t(s))\Big|_{t=0} s^2 t + \frac{\partial}{\partial s}(\nu(s)k_s(t))\Big|_{s=0} t^2 s + \left(\nu(s)k_s(t) - \nu(0)k_0(t) - \frac{\partial}{\partial s}(\nu(s)k_s(t))\Big|_{s=0} s\right)t^2. \tag{6.12}$$

The sum has been written (adding and subtracting the second terms of the second and third row) so that the first row contains the trivial terms and the second and third rows are symmetric in the two variables (that is, they are invariant under interchanges of s and t, h and k, and n and ν). The corresponding form for f given by (6.11) and (6.9) differs from (6.12) only in the final summand. The equality of the two forms is therefore equivalent to the equation

$$\left(\nu(s)k_s(t) - \nu(0)k_0(t) - \frac{\partial}{\partial s}(\nu(s)k_s(t))\Big|_{s=0} s\right)t^2 = \left(n(t)h_t(s) - n(0)h_0(s) - \frac{\partial}{\partial t}(n(t)h_t(s))\Big|_{t=0} t\right)s^2. \tag{6.13}$$

It now follows, by (6.13) and C(1), (C2), (C9), (C0) and (C5), that

$$\frac{s^2}{2}\frac{\partial^2}{\partial t^2}(n(t)h_t(s))\Big|_{t=0} = \lim_{t\to 0}\frac{1}{t^2}\left(n(t)h_t(s) - n(0)h_0(s) - \frac{\partial}{\partial t}(n(t)h_t(s))\Big|_{t=0} t\right)s^2$$
$$= \lim_{t\to 0}\left(\nu(s)k_s(t) - \nu(0)k_0(t) - \frac{\partial}{\partial s}(\nu(s)k_s(t))\Big|_{s=0} s\right) = \nu(s) - \nu(0) - \nu'(0)s$$

and so

$$\nu(s) = \nu(0) + \nu'(0)s + \frac{s^2}{2}\frac{\partial^2}{\partial t^2}(n(t)h_t(s))\Big|_{t=0} \tag{6.14}$$

It follows from 6.14, by (C9) and (C0)–(C2), that $\nu''(0) = n''(0)$.

Now, by (6.14), using (6.5),

$$\nu(s)k_s(t) - \nu(0)k_0(t) - \frac{\partial}{\partial s}(\nu(s)k_s(t))\Big|_{s=0} s \tag{6.15}$$
$$= \left(\nu(0) + \nu'(0)s + \frac{s^2}{2}\frac{\partial^2}{\partial t^2}(n(t)h_t(s))\Big|_{t=0}\right)k_s(t) - \nu(0)k_0(t) - \frac{\partial}{\partial s}(\nu(s)k_s(t))\Big|_{s=0} s$$
$$= \nu(0)\left(k_s(t) - k_0(t) - \frac{\partial}{\partial s}k_s(t)\Big|_{s=0} s\right) + \nu'(0)s(k_s(t) - k_0(t))$$
$$+\frac{s^2}{2}\left(n(0)\frac{\partial^2}{\partial t^2}h_t(s)\Big|_{t=0} + 2n'(0)\frac{\partial}{\partial t}h_t(s)\Big|_{t=0} + n''(0)h_0(s)\right)k_s(t)$$
$$= \left(\Gamma_0\Psi_2(s,t) + \Gamma_1\Psi_1(s,t) + \left(\frac{1}{2}\Sigma_0 H_2(s) + \Sigma_1 H_1(s) + \frac{1}{2}Gh_0(s)\right)k_s(t)\right)s^2.$$

Using the corresponding formula for the right hand side of (6.13) we deduce that (6.13) is equivalent to (6.4). Substitution from (6.15) into (6.12) gives f in the final form (6.3). The proof of Theorem 6.1 is complete.

Theorem 6.4 below shows that the smooth solutions to equations (5.1) and (5.2) form essentially one three-parameter family. First we describe it.

For $(\alpha, \beta, e) \in \mathbb{R}^3$ let $D : [-1,1]^2 \to \mathbb{R}$ be the function defined by

$$D = 1 - \alpha s - \beta t + est.$$

Our concern is with the application of Theorem 6.1 to functions

$$\begin{aligned} h_t(s) &= \frac{1-\beta t}{D} = \frac{1}{1-(\alpha - et)s/(1-\beta t)}, \\ k_s(t) &= \frac{1-\alpha s}{D} = \frac{1}{1-(\beta - es)t/(1-\alpha s)}. \end{aligned} \tag{6.16}$$

The condition which (α, β, e) must satisfy in order that these functions be defined on the open square $(-1,1)^2$ is given by the next elementary proposition, whose proof is omitted.

PROPOSITION 6.2. *The three conditions*

(i) $D(s,t) = 1 - \alpha s - \beta t + est > 0$, *for all* $(s,t) \in (-1,1)^2$,
(ii) $D(s,t) = 1 - \alpha s - \beta t + est \geq 0$, *for all* $(s,t) \in [-1,1]^2$, *and*
(iii) $|\alpha + \beta| - 1 \leq e \leq 1 - |\alpha - \beta|$,

are equivalent. If condition (iii) *is satisfied then* $\max\{|\alpha|, |\beta|\} \leq 1$.

If $|\alpha| \leq |\beta| \neq 0$ *then condition* (iii) *is equivalent to*

(iv) $|e - \alpha\beta/|\beta|| \leq 1 - |\beta|$.

Throughout the subsequent discussion (α, β, e) will always denote a triple which satisfies condition (i) of the proposition.

If $h_t(s)$ and $k_s(t)$ are functions of the form (6.16) then the Assumptions (C0)–(C5) are satisfied and one calculates that

$$\begin{aligned} &\Phi_1(t,s) - k_s(t)H_1(s) = 0, \quad \Phi_2(t,s) - \tfrac{1}{2}k_s(t)H_2(s) = 0, \\ &\Psi_1(s,t) - h_t(s)K_1(t) = 0, \quad \Psi_2(s,t) - \tfrac{1}{2}h_t(s)K_2(t) = 0, \end{aligned}$$

and

$$k_s(t)h_0(s) = 1/D = h_s(t)k_0(t),$$

so that, for these functions, (6.4) places no restriction on the coefficients Δ, Σ_0, Σ_1, Γ_0, Γ_1 and G. Thus Thm. 6.1 has the following immediate corollary.

COROLLARY 6.3. *A function* $f : (-1,1)^2 \to \mathbb{R}$ *can be written both in the form*

$$f(s,t) = \lambda(s) + \mu(s)t + \nu(s)t^2 \frac{1-\alpha s}{1-\alpha s - \beta t + est} \tag{6.17}$$

and in the form

$$f(s,t) = l(t) + m(t)s + n(t)s^2 \frac{1-\beta t}{1-\alpha s - \beta t + est} \tag{6.18}$$

if and only if it is of the form

$$f(s,t) = A + Bs + Ct + \Delta st + \frac{(\Sigma_0 + \Sigma_1 t)(1-\beta t)s^2 + (\Gamma_0 + \Gamma_1 s)(1-\alpha s)t^2 + \frac{1}{2}Gs^2t^2}{1-\alpha s - \beta t + est},$$

which can also be written as

$$f(s,t) = A + Bs + Ct + \frac{\Delta st + (\Sigma_0 + \Sigma_1' t)s^2 + (\Gamma_0 + \Gamma_1' s)t^2 + G' s^2 t^2}{1 - \alpha s - \beta t + est}. \tag{6.19}$$

The two forms for f are related by the equations

$$\Sigma_1' = \Sigma_1 - \Sigma_0\beta - \Delta\alpha, \quad \Gamma_1' = \Gamma_1 - \Gamma_0\alpha - \Delta\beta, \quad G' = \tfrac{1}{2}G - \beta\Sigma_1 - \alpha\Gamma_1 + \Delta e.$$

Calculations in Section 7 will use the form (6.19) and the primes will be dropped from the Σ_1', Γ_1' and G'.

Definition. For $(\alpha, \beta, e) \in \mathbb{R}^3$ satisfying condition (i) of Prop. 6.2 let $F(\alpha, \beta, e)$ be the set of those functions of the form (6.19) which are operator convex. Then $F(\alpha, \beta, e)$ is a finite-dimensional convex cone which contains $\mathcal{L}_2$. That it is often non-trivial will be seen in Section 8, which is devoted to an investigation of the sets $F(\alpha, \beta, e)$. Cor. 6.3 has as a consequence the following result.

Theorem 6.4. *For each (α, β, e) the set $F(\alpha, \beta, e)$ is a face of the convex cone $\mathcal{OC}_2$.*

Proof. Suppose that $f \in F(\alpha, \beta, e)$, that $f_0, f_1 \in \mathcal{OC}_2$, $0 < \theta < 1$ and that $f = (1-\theta)f_0 + \theta f_1$. The function f can be represented in each of the forms (6.17) and (6.18), and so also in the forms (5.1) and (5.2) with

$$\alpha(t) = \frac{\alpha - et}{1 - \beta t}, \quad \beta(s) = \frac{\beta - et}{1 - \alpha s}.$$

Thus for each $s \in (-1, 1)$ the function $f(s, \cdot)$ and for each $t \in (-1, 1)$ the function $f(\cdot, t)$ are extremal functions of $\mathcal{OC}_1$. Therefore f_0 and f_1 are also of the form (6.17) and of the form (6.18). Then, by Cor. 6.3, they are also of the form (6.19) and so lie in $F(\alpha, \beta, e)$. This shows that $F(\alpha, \beta, e)$ is an extremal subset of $\mathcal{OC}_2$; it is also closed and convex and so is a face of $\mathcal{OC}_2$.

The next theorem shows that the functions of Cor. 6.3 provide the only nice solutions to equations (5.1) and (5.2).

Theorem 6.5. *If $f : (-1, 1)^2 \to \mathbb{R}$ is a function, not of the form $f(s,t) = A + Bs + Ct + \Delta st$, which has representations*

$$f(s,t) = \lambda(s) + \mu(s)t + \nu(s)\frac{t^2}{1 - \beta(s)t} \tag{6.20}$$

and

$$f(s,t) = l(t) + m(t)s + n(t)\frac{s^2}{1 - \alpha(t)s} \tag{6.21}$$

in which the functions $\alpha(t)$ and $\beta(s)$ have continuous second derivatives, then for some $(\alpha, \beta, e) \in \mathbb{R}^3$ the function $f(s,t)$ is of the form

$$f(s,t) = A + Bs + Ct + \frac{\Delta st + (\Sigma_0 + \Sigma_1 t)s^2 + (\Gamma_0 + \Gamma_1 s)t^2 + Gs^2t^2}{1 - \alpha s - \beta t + est}, \tag{6.22}$$

where $A, B, C, \Delta, \Sigma_0, \Sigma_1, \Gamma_0, \Gamma_1, G \in \mathbb{R}$.

Proof. Write

$$h_t(s) = \frac{1}{1-\alpha(t)s}, \quad k_s(t) = \frac{1}{1-\beta(s)t}.$$

Then h and k satisfy conditions (C0)–(C5) and so, by Thm. 6.1, f is of the form (6.3), the cofficients $\Sigma_0, \Sigma_1, \Gamma_0, \Gamma_1$ and G are not all zero, and h, k satisfy the relation (6.4). Rearranging (6.4) so that $k_s(t)$, either explicitly or implicitly in Ψ_1 and Ψ_2, appears only on the left, and $h_t(s)$ appears only on the right, we obtain the equivalent relation

$$\begin{aligned}(6.23)\quad &\Gamma_0\Psi_2 + \Gamma_1\Psi_1 + \tfrac{1}{2}Gk_s(t)h_0(s) + \tfrac{1}{2}\Sigma_0 k_s(t)H_2(s) + \Sigma_1 k_s(t)H_1(s)\\ &= \Sigma_0\Phi_2 + \Sigma_1\Phi_1 + \tfrac{1}{2}Gh_t(s)k_0(t) + \tfrac{1}{2}\Gamma_0 h_t(s)K_2(t) + \Gamma_1 h_t(s)K_1(t).\end{aligned}$$

We now calculate the left and right hand sides of (6.23) in terms of the functions $\alpha(t)$ and $\beta(s)$ explicitly. Let

$$R_l(s) = \frac{\Gamma_0}{s^2} + \frac{\Gamma_1}{s} + \frac{1}{2}Gh_0(s) + \frac{1}{2}\Sigma_0 H_2(s) + \Sigma_1 H_1(s)$$

(the subscript "l" in R_{l} is for "left"). Then

$$R_{\mathrm{l}}(s) = \frac{1}{(1-\alpha(0)s)^3 s^2}\varrho_{\mathrm{l}}(s),$$

where $\varrho_{\mathrm{l}}(s)$ is a polynomial. Let

$$Q_{\mathrm{l}}(s,t) = \frac{\Gamma_0}{s^2}\left(k_0(t) + K_1(t)s\right) + \frac{\Gamma_1}{s}k_0(t).$$

Then

$$Q_{\mathrm{l}}(s,t) = \frac{1}{s^2(1-\beta(0)t)^2}Q'_{\mathrm{l}}(s,t)$$

where $Q'_{\mathrm{l}}(s,t) = (\Gamma_0 + \Gamma_1 s)(1-\beta(0)t) + \Gamma_0\beta'(0)st$ is a polynomial, of degree at most one in each of s and t. The left hand side of (6.23) is $k_s(t)R_{\mathrm{l}}(s) - Q_{\mathrm{l}}(s,t)$. There are corresponding functions and polynomials for the right hand side of (6.23) (with subscript "r" for "right") and the equation can now be written as

$$(6.24)\qquad k_s(t)R_{\mathrm{l}}(s) - Q_{\mathrm{l}}(s,t) = h_t(s)R_{\mathrm{r}}(t) - Q_{\mathrm{r}}(t,s).$$

If R_{l} is zero then $\Gamma_0 = \Gamma_1 = G = 0$. Therefore, by the assumption that f is non-trivial, R_{l} and R_{r} are not both zero. There is a symmetry between the left and right of (6.24) and we may assume that R_{l} is non-zero. From (6.24) it follows that

$$k_s(t) = \frac{h_t(s)R_{\mathrm{r}}(t) - Q_{\mathrm{r}}(t,s) + Q_{\mathrm{l}}(s,t)}{R_{\mathrm{l}}(s)}$$

and

$$(6.25)\qquad \beta(s) = \frac{1}{t}\left(1 - \frac{1}{k_s(t)}\right) = \frac{(1/t)(h_t(s)R_{\mathrm{r}}(t) - Q_{\mathrm{r}}(t,s) + Q_{\mathrm{l}}(s,t) - R_{\mathrm{l}}(s))}{h_t(s)R_{\mathrm{r}}(t) - Q_{\mathrm{r}}(t,s) + Q_{\mathrm{l}}(s,t)}$$

Equation (6.25) holds for all $s, t \in (-1,1)\setminus\{0\}$, so $\beta(s)$ is the limit as $t \to 0$ of the right hand side of (6.25). It follows that $R_{\mathrm{l}}(s)$ is the limit as $t \to 0$ of the denominator on the right of (6.25) and that the numerator is convergent to a limit $L_\beta(s)$, say. Then substituting for R_{r}, Q_{r}, Q_{l} and R_{l}, we obtain

$$L_\beta(s) = \lim_{t\to 0} \Sigma_0 \frac{1}{t^3}\left(h_t(s) - h_0(s) - H_1(s)t - \frac{1}{2}H_2(s)t^2\right)$$
$$+\Sigma_1 H_2(s) + \beta'(0)\left(\frac{\Gamma_0}{s} + \Gamma_1 h_0(s)\right) + \beta''(0)\tfrac{1}{2}h_0(s)\Gamma_0 + \frac{G}{2}\left(H_1(s) + h_0(s)\beta(0)\right).$$

The limit on the right (the first term of the sum) must exist and it follows (by laborious calculation) that if $\Sigma_0 \neq 0$ then

$$\lim_{t\to 0} \frac{1}{t^3}\left(\alpha(t) - \alpha(0) - \alpha'(0)t - \frac{1}{2}\alpha''(0)t^2\right)$$

exists and that, whatever Σ_0,

$$L_\beta(s) = \frac{1}{(1-\alpha(0)s)^4 s^2} P_\beta(s) \tag{6.26}$$

where P_β is a polynomial. Thus, taking the limit as $t \to 0$ in (6.25) we obtain the following expressions for $\beta(s)$ and $k_s(t)$:

$$\beta(s) = \frac{L_\beta(s)}{R_{\mathrm{l}}(s)} = \frac{P_\beta(s)}{(1-\alpha(0)s)\varrho_{\mathrm{l}}(s)}, \quad k_s(t) = \frac{(1-\alpha(0)s)\varrho_{\mathrm{l}}(s)}{(1-\alpha(0)s)\varrho_{\mathrm{l}}(s) - P_\beta(s)t}. \tag{6.27}$$

In particular, $\beta(s)$ is a rational function. Note that the denominator in the expression for $k_s(t)$ is never zero.

If $R_{\mathrm{r}} \neq 0$ then there are corresponding expressions for $\alpha(t)$ and $h_t(s)$ for which a symmetric notation will be used: $P_\alpha(t)$, $\varrho_{\mathrm{r}}(t)$ and $Q'_{\mathrm{r}}(t,s)$.

Let $M_{\mathrm{l}}(s)$ be a greatest common divisor of the polynomials $(1-\alpha(0)s)\varrho_{\mathrm{l}}(s)$ and $P_\beta(s)$. If $(1-\beta(0)t)\varrho_{\mathrm{r}}(t)$ and $P_\beta(s)$ are not both zero let $M_{\mathrm{r}}(t)$ be a greatest common divisor. Let

$$\Pi_{\mathrm{l}}(s,t) = \frac{(1-\alpha(0)s)\varrho_{\mathrm{l}}(s)}{M_{\mathrm{l}}(s)} - \frac{P_\beta(s)}{M_{\mathrm{l}}(s)}t, \quad \Pi_{\mathrm{r}}(t,s) = \frac{(1-\beta(0)t)\varrho_{\mathrm{r}}(t)}{M_{\mathrm{r}}(t)} - \frac{P_\alpha(t)}{M_{\mathrm{r}}(t)}s.$$

There are now two cases to be considered.

CASE 1: $R_{\mathrm{l}} \neq 0$, $R_{\mathrm{r}} = 0$. In this case $\Sigma_0 = \Sigma_1 = G = 0$. The relation (6.24) becomes, on substituting for $k_s(t)$ from (6.27),

$$t^2\varrho_{\mathrm{l}}(s)^2(1-\beta(0)t)^2 = M_{\mathrm{l}}(s)\Pi_{\mathrm{l}}(s,t)(Q'_{\mathrm{l}}(s,t)t^2(1-\alpha(0)s)^2 - Q'_{\mathrm{r}}(t,s)s^2(1-\beta(0)t)^2) \tag{6.28}$$

If $P_\beta = 0$ then $\beta(s) = 0 = \beta(0)$. Suppose $P_\beta \neq 0$. If the second factor on the right of (6.28) is of degree zero in s then, by (6.27), $\beta(s) = \beta(0)$; if it were of degree ≥ 1 in s then it would be an irreducible polynomial in the unique factorisation domain $\mathbb{R}[s,t]$ and would consequently divide one of the factors on the left of (6.28), which is not possible. Therefore $\beta(s) = \beta(0)$ and, if we put $\beta = \beta(0)$, $k_s(t) = (1-\beta t)^{-1}$. Then by (6.3), $f(s,t)$ is of the form

$$f(s,t) = A + Bs + Ct + \Delta st + (\Gamma_0 t^2 + \Gamma_1 st^2)\frac{1}{1-\beta t}$$

and is linear as a function of s. The function $\alpha(t)$ is indeterminate but does not enter into the representation (6.21). The representation (6.22) holds with $(\alpha,\beta,e) = (0,\beta,0)$.

CASE 2: $R_l \neq 0,\ R_r \neq 0$. It will be shown that in this case

$$\beta(s) = \beta(0) + \frac{ds}{1-\alpha(0)s}, \quad \alpha(t) = \alpha(0) + \frac{dt}{1-\beta(0)t} \tag{6.29}$$

where $d = \alpha'(0) = \beta'(0)$, so that, by (6.19) of Cor. 6.3, the conclusion of the theorem is satisfied by $(\alpha, \beta, e) = (\alpha(0), \beta(0), \alpha(0)\beta(0) - d)$.

It follows from the conditions of Case 2 that $\varrho_l \neq 0$ and $\varrho_r \neq 0$. The functions $\beta(s)$ and $\alpha(t)$, $k_s(t)$ and $h_t(s)$, are given by (6.27) and the corresponding right hand version. The relation (6.24), on substituting for $k_s(t)$ and $h_t(s)$, becomes

$$\begin{aligned} &\varrho_l(s)^2(1-\beta(0)t)^2t^2M_r(t)\Pi_r(t,s) - \varrho_r(t)^2(1-\alpha(0)s)^2s^2M_l(s)\Pi_l(s,t) \\ &\quad = M_r(t)\Pi_r(t,s)M_l(s)\Pi_l(s,t)(Q_l'(s,t)t^2(1-\alpha(0)s)^2 - Q_r'(t,s)s^2(1-\beta(0)t)^2), \end{aligned} \tag{6.30}$$

which is a polynomial identity.

There are now three subcases to be considered.

(a) Suppose $P_\beta(s) = 0,\ P_\alpha(t) = 0$. Then $\beta(s) = 0,\ \alpha(t) = 0$ and the equalities (6.29) are satisfied.

(b) Suppose $P_\beta(s) = 0,\ P_\alpha(t) \neq 0$. Then $\beta(s) = 0$ and $k_s(t) = 1$. The identity (6.30) becomes

$$\begin{aligned} &\varrho_l(s)t^2M_r(t)\Pi_r(t,s) - \varrho_r(t)^2(1-\alpha(0)s)^3s^2 \\ &\quad = M_r(t)\Pi_r(t,s)(1-\alpha(0)s)(Q_l'(s,t)t^2(1-\alpha(0)s)^2 - Q_r'(t,s)s^2). \end{aligned}$$

Then $\Pi_r(t,s)$ is an irreducible polynomial in $\mathbb{R}[s,t]$ and is a divisor of the second summand on the left; it has to be an associate of $(1-\alpha(0)s)$:

$$\frac{\varrho_r(t)}{M_r(t)} - \frac{P_\alpha(t)}{M_r(t)}s = \theta(1-\alpha(0)s)$$

for some $\theta \in \mathbb{R}$. It follows that $\alpha(t) = \alpha(0)$. Thus the equalities (6.29) are again satisfied.

(c) Now suppose that $P_\beta(s) \neq 0,\ P_\alpha(t) \neq 0$. Let δ_l be the degree in s of $\Pi_l(s,t)$; its degree in t is one.

If $\delta_l \geq 1$ then $\Pi_l(s,t)$ is an irreducible polynomial in $\mathbb{R}[s,t]$, it is a divisor of two of the products in (6.30), so is a divisor of the third, in which only the factor $\Pi_r(s,t)$ can be of positive degree in both s and t. The factor $\Pi_r(s,t)$ is also irreducible and therefore $\Pi_r(s,t)$ and $\Pi_l(s,t)$ are associates:

$$\frac{(1-\alpha(0)s)\varrho_l(s)}{M_l(s)} - \frac{P_\beta(s)}{M_l(s)}t = \theta\left(\frac{(1-\beta(0)t)\varrho_r(t)}{M_r(t)} - \frac{P_\alpha(t)}{M_r(t)}s\right) \tag{6.31}$$

for some $\theta \in \mathbb{R} \setminus \{0\}$. It follows that $\Pi_l(s,t)$ and $\Pi_r(t,s)$ are in this case both of degree one in each of s and t. Thus

$$\begin{aligned} \frac{(1-\alpha(0)s)\varrho_l(s)}{M_l(s)} &= x_{l1} + x_{l2}s, \quad \frac{P_\beta(s)}{M_l(s)} = y_{l1} + y_{l2}s, \\ \frac{(1-\beta(0)t)\varrho_r(t)}{M_r(t)} &= x_{r1} + x_{r2}t, \quad \frac{P_\alpha(t)}{M_r(t)} = y_{r1} + y_{r2}t \end{aligned}$$

for some constants $x_{l1}, x_{l2}, \ldots$ Then by (6.27) and its companion

$$\beta(s) = \frac{y_{l1} + y_{l2}s}{x_{l1} + x_{l2}s}, \quad \alpha(t) = \frac{y_{r1} + y_{r2}t}{x_{r1} + x_{r2}t},$$

and, by equating coefficients in (6.31),

$$x_{l1} = \theta x_{r1}, \quad x_{l2} = -\theta y_{r1}, \; y_{l1} = -\theta x_{r2}, \quad y_{l2} = \theta y_{r2}.$$

It follows that

$$\beta(s) = \frac{-x_{r2} + y_{r2}s}{x_{r1} - y_{r1}s}, \quad \beta(0) = -\frac{x_{r2}}{x_{r1}}, \quad \alpha(0) = \frac{y_{r1}}{x_{r1}},$$

and the equations (6.29) are satisfied by $d = \alpha(0)\beta(0) + y_{r2}/x_{r1}$. It follows that $d = \alpha'(0) = \beta'(0)$.

Suppose finally that $\delta_l = 0$. If δ_r, the degree of $\Pi_r(t,s)$ in t, were at least one then it would follow, as in the previous case, that $\delta_l \geq 1$. So $\Pi_l(s,t)$ is of degree zero in s and $\Pi_r(t,s)$ is of degree zero in t. Consequently, $\beta(s) = \beta(0)$ and $\alpha(t) = \alpha(0)$ and the equalities (6.29) are again satisfied.

The proof of Theorem 6.5 is complete.

REMARK. Suppose now that $f \in \mathcal{OC}_2$ and that for each s the function $f(s,\cdot)$ and for each t the function $f(\cdot,t)$ are extremal in $\mathcal{OC}_1$. Then f can be represented in each of the forms (5.1) and (5.2). If the functions $\alpha(t)$ and $\beta(s)$ which occur are twice continuously differentiable then the hypotheses of Thm. 6.5 are satisfied and therefore f is of the form (6.19) for some $(\alpha,\beta,e) \in \mathbb{R}^3$. However, in the representation (5.1), $\lambda(s) = f(s,0)$, $\mu(s) = f^{(0,1)}(s,0)$ and $\nu(s) = \frac{1}{2}f^{(0,2)}(s,0)$. If $f^{(0,2)}(s,0)$ is nowhere zero then $\beta(s)$ can be expressed in terms of f and its derivatives, and if these are sufficiently differentiable then $\beta(s)$ will be twice continuously differentiable.

In Section 7 those functions of the form (6.19) which are operator convex will be characterised. In Section 8 the faces $F(\alpha,\beta,e)$ of $\mathcal{OC}_2$ will be described.

7. A characterisation of functions in $F(\alpha,\beta,e)$

Suppose that $f : (-1,1)^2 \to \mathbb{R}$ is a function of the form (6.19):

$$f(s,t) = A + Bs + Ct + \frac{\Delta st + (\Sigma_0 + \Sigma_1 t)s^2 + (\Gamma_0 + \Gamma_1 s)t^2 + Gs^2t^2}{D(s,t)} \tag{7.1}$$

where $D(s,t) = 1 - \alpha s - \beta t + est$ and (α,β,e) satisfies the condition of Prop. 6.2. Then $f \in C^2((-1,1)^2)$, by Thm. 4.2 the operator function f is also a C^2 function, and so, by Thm. 3.2, $f \in \mathcal{OC}_2$ if and only if $d^2f(A,B)(H,K)^2 \geq 0$ for all $(A,B) \in \mathcal{S}_I(\mathbb{C}^M) \times \mathcal{S}_I(\mathbb{C}^N)$, for all $(H,K) \in \mathcal{S}(\mathbb{C}^M) \times \mathcal{S}(\mathbb{C}^N)$ and all $M,N \in \mathbb{N}$. The operator $f(A+H, B+K)$ has a series expansion as a sum of terms each of which is homogeneous in (H,K). The operator $\frac{1}{2}d^2f(A,B)(H,K)^2$ is the sum of those terms which are homogeneous of degree two. However, this procedure, or, alternatively, the use of extensions of the elementary rules of the calculus, yields a formula for $d^2f(A,B)(H,K)^2$ which is not apparently self-adjoint. The formula, in order to be tractable, must be recast. We do not have an algorithm for doing so. The formula (7.2) below was initially found by direct, exploratory and lengthy calculations which, with hindsight, it is possible to abbreviate.

In the statement and proof of the next theorem the following notation will be used. If P is an operator then $\{P + *\}$ will denote the sum $P + P^*$ of P and its adjoint. In terms which are of the form $D(A,B), p(A,B), \frac{\partial p}{\partial s}(A,B), \ldots$ the operator variables A and B may be suppressed and we will write simply $D, P, \frac{\partial p}{\partial s}, \ldots$ It will be clear from the context whether the arguments of $D, P, \frac{\partial p}{\partial s}, \ldots$ are to be read as (A,B) or (s,t).

THEOREM 7.1. *Suppose* $f : (-1,1)^2 \to \mathbb{R}$ *is a function of the form* (7.1)*. Then*

$$\begin{aligned}(7.2)\quad & D\frac{1}{2}d^2 f(A,B)(H,K)^2 D \\ &= H\otimes I\, I\otimes S_1(B)\, D^{-1}\, H\otimes I + I\otimes K\, S_2(A)\otimes I\, D^{-1}\, I\otimes K \\ &\quad + \{H\otimes I\, S(A,B)D^{-1}\, I\otimes K + *\} \\ &\quad - (\Sigma_0 e + \Sigma_1\alpha)A\otimes I\, H\otimes K\, A\otimes I - (\Gamma_0 e + \Gamma_1\beta) I\otimes B\, H\otimes K\, I\otimes B \\ &\quad + G\Big\{A\otimes B\, H\otimes K\left(D - \frac{e}{2}A\otimes B\right) + *\Big\},\end{aligned}$$

where the functions S_1, S_2, *and* S *are given by*

$$(7.3)\qquad S_1(t) = \frac{1}{2}D^3\frac{\partial^2 f}{\partial s^2}(s,t), \quad S_2(s) = \frac{1}{2}D^3\frac{\partial^2 f}{\partial t^2}(s,t)$$

and

$$S(s,t) = \frac{1}{2}D^3\frac{\partial^2 f}{\partial s\partial t} + \frac{D}{2}(\Sigma_0 e + \Sigma_1\alpha)s^2 + \frac{D}{2}(\Gamma_0 e + \Gamma_1\beta)t^2 - GDst\left(D - \frac{1}{2}est\right).$$

PROOF. Let p denote the numerator of the quotient in (7.1). It is a polynomial in s and t of degree at most two in each of s and t. The second Fréchet derivatives of the operator functions f and pD^{-1} coincide.

First consider the derivatives of the operator function p. If $q(s)$ is one of the functions $1, s$ and s^2 then

$$(7.4)\qquad q(A+H) = q(A) + \left\{\frac{1}{2}\frac{\partial q}{\partial s}(A)H + *\right\} + \frac{1}{2}\frac{\partial^2 q}{\partial s^2}(A)H^2.$$

If $r(t)$ is one of the functions $1, t, t^2$ and $p = qr$ then $p(A+H, B+K) = q(A+H)\otimes r(B+K)$ and, substituting for $q(A+H)$ from (7.4) and for $r(B+K)$ from the corresponding equation, one obtains the equation

$$\begin{aligned}(7.5)\quad p(A+H,B+K) &= p + \left\{\left(\frac{1}{2}\frac{\partial p}{\partial s}H\otimes I + \frac{1}{2}\frac{\partial p}{\partial t}I\otimes K\right) + *\right\} \\ &\quad + \frac{1}{2}\frac{\partial^2 p}{\partial s^2}H^2\otimes I + \frac{1}{2}\frac{\partial^2 p}{\partial t^2}I\otimes K^2 \\ &\quad + \left\{\frac{1}{4}\frac{\partial^2 p}{\partial s\partial t}H\otimes K + *\right\} + \left\{\frac{1}{4}H\otimes I\,\frac{\partial^2 p}{\partial s\partial t}\,I\otimes K + *\right\} \\ &\quad + \text{ terms of higher degree in } (H,K).\end{aligned}$$

The equation (7.5) extends by linearity to any polynomial p of degree at most two in each of s and t.

One can write

$$D(A+H,B+K)=D+\frac{\partial D}{\partial s}\,H\otimes I+\frac{\partial D}{\partial t}\,I\otimes K+eH\otimes K,$$

and a geometric series expansion of $D(A+H,B+K)^{-1}$ gives the equation

$$\begin{aligned}(7.6)\quad D^{-1}(A+H,B+K)=D^{-1}-D^{-1}\Big(\frac{\partial D}{\partial s}\,H\otimes I+\frac{\partial D}{\partial t}\,I\otimes K\Big)D^{-1}\\ +D^{-1}\Big(\frac{\partial D}{\partial s}\Big)^2 H\otimes I\,D^{-1}\,H\otimes I\,D^{-1}\\ +D^{-1}\Big(\frac{\partial D}{\partial t}\Big)^2 I\otimes K\,D^{-1}\,I\otimes K\,D^{-1}\\ +D^{-1}\Big(\Big\{H\otimes I\frac{\partial D}{\partial s}\frac{\partial D}{\partial t}D^{-1}\,I\otimes K+*\Big\}-eH\otimes K\Big)D^{-1}\\ +\text{ terms of higher degree in }(H,K).\end{aligned}$$

Now $\frac{1}{2}d^2(pD^{-1})(A,B)(H,K)^2$ is the sum of terms of degree two in (H,K) in the expansion of the product $p(A+H,B+K)D^{-1}(A+H,B+K)$, where the factors are replaced by the expressions of (7.5) and (7.6). Thus

$$(7.7)\qquad D\tfrac{1}{2}d^2f(A,B)(H,K)^2D=T_{11}+T_{22}+T_{12}$$

where T_{11} and T_{22} are the sums of those terms which are of degree two in H and K respectively, and T_{12} is the sum of those terms which are of degree one in each of H and K. The first two of these summands are easily dealt with:

$$\begin{aligned}T_{11}=\Big[p\Big(\frac{\partial D}{\partial s}\Big)^2-D\frac{1}{2}\frac{\partial p}{\partial s}\frac{\partial D}{\partial s}\Big]H\otimes I\,D^{-1}\,H\otimes I\\ +D\,H\otimes I\Big[\frac{1}{2}\frac{\partial^2 p}{\partial s^2}D-\frac{1}{2}\frac{\partial p}{\partial s}\frac{\partial D}{\partial s}\Big]D^{-1}\,H\otimes I.\end{aligned}$$

The derivative with respect to s of the function of the second square bracket on the right is zero, so the function is a function of t alone, and the term in square brackets commutes with $H\otimes I$. So

$$T_{11}=\Big[p\Big(\frac{\partial D}{\partial s}\Big)^2-D\frac{1}{2}\frac{\partial p}{\partial s}\frac{\partial D}{\partial s}+\frac{1}{2}\frac{\partial^2 p}{\partial s^2}D^2-\frac{1}{2}\frac{\partial p}{\partial s}\frac{\partial D}{\partial s}D\Big]H\otimes I\,D^{-1}\,H\otimes I.$$

The derivative of the function of the term in square brackets with respect to s is zero, so the function is a function of t alone, and we will denote it by $S_1(t)$. The term in square brackets is then $I\otimes S_1(B)$ and it commutes with $H\otimes I$. Therefore

$$T_{11}=H\otimes I\,I\otimes S_1(B)\,D^{-1}\,H\otimes I,$$

and there is a corresponding form for T_{22}.

The summand T_{12} is a sum of eleven terms, each a product; we can write

$$T_{12}=T_{12}^{(1)}+T_{12}^{(2)}+T_{12}^{(3)}$$

where

$$
\begin{aligned}
T_{12}^{(1)} &= p\,H\otimes I\,\frac{\partial D}{\partial s}\frac{\partial D}{\partial t}D^{-1}\,I\otimes K \\
&\quad -\frac{1}{2}D\frac{\partial p}{\partial s}\,H\otimes I\,\frac{\partial D}{\partial t}D^{-1}\,I\otimes K-\frac{1}{2}D\,H\otimes I\,\frac{\partial p}{\partial s}\frac{\partial D}{\partial t}D^{-1}\,I\otimes K, \\
T_{12}^{(2)} &= p\,I\otimes K\,\frac{\partial D}{\partial s}\frac{\partial D}{\partial t}D^{-1}\,H\otimes I \\
&\quad -\frac{1}{2}D\frac{\partial p}{\partial t}\,I\otimes K\,\frac{\partial D}{\partial s}D^{-1}\,H\otimes I-\frac{1}{2}D\,I\otimes K\,\frac{\partial p}{\partial t}\frac{\partial D}{\partial s}D^{-1}\,H\otimes I, \\
T_{12}^{(3)} &= -ep\,H\otimes K+D\bigg[\bigg\{\frac{1}{4}\frac{\partial^2 p}{\partial s\partial t}\,H\otimes K+*\bigg\}+\bigg\{H\otimes I\,\frac{1}{4}\frac{\partial^2 p}{\partial s\partial t}\,I\otimes K+*\bigg\}\bigg].
\end{aligned}
$$

In the course of the reduction of T_{12} to the form stated in the theorem bookkeeping is not necessary for terms of the form $H\otimes I\,\Phi(A,B)\,I\otimes K$ or $I\otimes K\,\Psi(A,B)\,H\otimes I$. A sum of such terms will be denoted by (BIN).

The function $p(s,t)$ can be written as

$$p(s,t)=\tau_0+\tau_1 s+\tau_2 s^2=\sigma_0+\sigma_1 t+\sigma_2 t^2$$

where $\tau_0,\ \tau_1,\ \tau_2$ and $\sigma_0,\ \sigma_1,\ \sigma_2$ are quadratic functions of t and s respectively. One can write

$$D=I\otimes(I-\beta B)+A\otimes I\,\frac{\partial D}{\partial s} \tag{7.8}$$

and so

$$D\,H\otimes I=H\otimes I\,I\otimes(I-\beta B)+A\otimes I\,H\otimes I\,\frac{\partial D}{\partial s}. \tag{7.9}$$

If, now, in the expression for $T_{12}^{(1)}$ one substitutes for p and $\frac{\partial p}{\partial s}$ in terms of τ_0,τ_1,τ_2, for D in the second term from (7.8), and for $D\,H\otimes I$ in the third term from (7.9), and expands the products then the term involving τ_0 and three of the terms involving $I-\beta B$ can be assigned to (BIN), the terms involving τ_1 and $A^2\otimes\tau_2$ cancel, and the remaining two terms combine (going from right to left in (7.8)) to give the equation

$$T_{12}^{(1)}=A\otimes\tau_2(B)\,H\otimes K\,(\beta I-eA)\otimes I+(\mathrm{BIN}). \tag{7.10}$$

In a similar way one obtains the equation

$$T_{12}^{(2)}=\sigma_2(A)\otimes B\,H\otimes K\,I\otimes(\alpha I-eB)+(\mathrm{BIN}). \tag{7.11}$$

Now suppose that $p(s,t)=s^k t^l$. Then

$$
\begin{aligned}
T_{12}^{(3)} &= \frac{kl}{4}D(A,B)\{A^{k-1}\otimes B^{l-1}\,H\otimes K+*\} \\
&\quad +\frac{kl}{4}D(A,B)\{I\otimes B^{l-1}\,H\otimes K\,A^{k-1}\otimes I+*\}-eA^k\otimes B^l\,H\otimes K.
\end{aligned} \tag{7.12}
$$

Substituting in turn $(k,l)=(1,1),(2,0),(0,2),(2,1),(1,2)$ and $(2,2)$, with the corresponding functions τ_2 and σ_2, one obtains from (7.10)–(7.12) a simple expression for T_{12} for each of the functions $p=st,s^2,t^2,s^2t,st^2$ and s^2t^2. Taking the linear combination for the general polynomial p of (7.1) one obtains the equation

$$T_{12} = (\mathrm{BIN}) - (\Sigma_0 e + \Sigma_1\alpha)\, A\otimes I\, H\otimes K\, A\otimes I - (\Gamma_0 e + \Gamma_1\beta)\, I\otimes B\, H\otimes K\, I\otimes B + G\Big\{A\otimes B\, H\otimes K\left(D - \frac{e}{2}A\otimes B\right) + *\Big\}. \tag{7.13}$$

However, the left hand side of (7.7) is self-adjoint and so also are T_{11} and T_{22}. Therefore T_{12} is self-adjoint and so the term (BIN) is self-adjoint. Thus (BIN) can be replaced by $\frac{1}{2}\{(\mathrm{BIN}) + *\}$ and hence T_{12} is obtained in the form implicit in (7.2). The form (7.2) is now established.

In the case in which $M = N = 1$ the equation (7.2) becomes, if we replace (A, B) by (s, t) and (H, K) by (h, k),

$$\begin{aligned} D\frac{1}{2}d^2 f(s,t)(h,k)^2 D &\\ = S_1(t)D^{-1}h^2 + S_2(s)D^{-1}k^2 &\\ + (2S(s,t)D^{-1} - (\Sigma_0 e + \Sigma_1\alpha)s^2 - (\Gamma_0 e + \Gamma_1\beta)t^2 + G(2D - est))hk, \end{aligned}$$

from which the expressions for S_1, S_2 and S follow. The proof of Theorem 7.1 is complete.

It is now possible to characterise those functions of the form (7.1) which are operator convex.

THEOREM 7.2. *Let* $f : (-1,1)^2 \to \mathbb{R}$ *be defined by equation* (7.1). *Then the following conditions are equivalent*:

(1) $f \in \mathcal{OC}_2$.
(2) $\Sigma_0 e + \Sigma_1\alpha = \Gamma_0 e + \Gamma_1\beta = G = 0$ *and* $f : (-1,1)^2 \to \mathbb{R}$ *is convex.*
(3) $\Sigma_0 e + \Sigma_1\alpha = \Gamma_0 e + \Gamma_1\beta = G = 0$ *and*

$$S_1(t) \ge 0, \quad S_2(s) \ge 0 \quad \text{and} \quad S_1(t)S_2(s) \ge S(s,t)^2$$

for all $(s,t) \in [-1,1]^2$, *where* S_1, S_2 *and* S *are the functions of Thm.* 7.1.

PROOF. By Thm. 4.2 the operator functions of f are infinitely differentiable and, by Thm. 3.2, $f \in \mathcal{OC}_2$ if and only if

$$D(A,B)\frac{1}{2}d^2 f(A,B)(H,K)^2 D(A,B) \ge 0 \tag{7.14}$$

for all $A \in \mathcal{S}_I(\mathbb{C}^M),\ B \in \mathcal{S}_I(\mathbb{C}^N)$, all $H \in \mathcal{S}(\mathbb{C}^M),\ K \in \mathcal{S}(\mathbb{C}^N)$ and all $M, N \in \mathbb{N}$.

Henceforth we will suppress the variables A, B and H, K in the expressions $S_1(B)$, $D(A,B), \ldots$ and write simply $S_1, D, \ldots$ when it is not inconvenient to do so.

(1)⇒(2). Suppose that $f \in \mathcal{OC}_2$. Condition (7.14) is equivalent to the condition that

$$\big\langle D\tfrac{1}{2}d^2 f D x, x\big\rangle \ge 0 \tag{7.15}$$

for all relevant A, B, H, K and all $x \in \mathbb{C}^M \otimes \mathbb{C}^N$ and all $M, N \in \mathbb{N}$.

Suppose that $\Sigma_0 e + \Sigma_1\alpha \ne 0$. It will be shown that the condition (7.15) is not satisfied. Let $B = 0$ and suppose that H, x have been chosen so that $H\otimes I x = 0$. Then

$$\begin{aligned} \big\langle D\tfrac{1}{2}d^2 f D x, x\big\rangle &= \langle S_2\otimes I\, D^{-1}\, I\otimes K x, I\otimes K x\rangle \\ &\quad - (\Sigma_0 e + \Sigma_1\alpha)\langle I\otimes K\, A\otimes I x, H\otimes I\, A\otimes I x\rangle. \end{aligned}$$

The first term on the right is of degree two in K, the second is of degree one. If for some choice of the variables the second term is non-zero then, replacing K by εK where ε is small and of appropriate sign, we obtain a choice which violates the condition (7.15). If $\xi_1, \xi_2 \in \mathbb{C}^M \setminus \{0\}$ is an orthonormal pair (so $M \geq 2$), $\eta \in \mathbb{C}^N \setminus \{0\}, x = \xi_1 \otimes \eta$, and $H \in \mathcal{S}(\mathbb{C}^M)$ is chosen so that $H\xi_1 = 0$ and $H\xi_2 = \xi_2$, $K = I \in \mathcal{S}(\mathbb{C}^N)$ and $A \in \mathcal{S}_I(\mathbb{C}^M)$ is chosen so that $A\xi_1 = \theta\xi_2$ where $0 < \theta < 1$ then

$$\langle I \otimes K\, A \otimes I\, x, H \otimes I\, A \otimes I\, x\rangle = \theta^2 \|\xi_2\|^2 \|\eta\|^2 \neq 0.$$

This proves that if $f \in \mathcal{OC}_2$ then $\Sigma_0 e + \Sigma_1 \alpha = 0$, and so, by symmetry, $\Gamma_0 e + \Gamma_1 \beta = 0$ also.

Now suppose that $f \in \mathcal{OC}_2$ and that $\Sigma_0 e + \Sigma_1 \alpha = \Gamma_0 e + \Gamma_1 \beta = 0$. Suppose that $G \neq 0$. It will be shown that the elements A, B, H, K and x can be chosen so that the condition (7.15) is violated.

Suppose that $\alpha \neq 0$. Again suppose that H, x have been chosen so that $H \otimes Ix = 0$. In this case

$$\begin{aligned}\left\langle D\frac{1}{2}d^2 f Dx, x\right\rangle = {}& \langle S_2 \otimes I\, D^{-1}\, I \otimes K\, x, I \otimes K\, x\rangle \\ & - 2\alpha G \operatorname{Re}\langle A \otimes B\, I \otimes K\, x, H \otimes I\, A \otimes I\, x\rangle \\ & + eG\langle A \otimes B\, H \otimes K\, A \otimes B\, x, x\rangle.\end{aligned}$$

The first term on the right is of degree two in K, the others are of degree one. So it is enough to show that the elements can be chosen so that the sum of the second and third terms is non-zero. But the second term is of degree one in B and the third is of degree two, so it is enough to show that the elements can be chosen so that

$$\operatorname{Re}\langle A \otimes B\, I \otimes K\, x, H \otimes I\, A \otimes I\, x\rangle \neq 0.$$

This is achieved by choosing $B = \phi I$ with $0 < \phi < 1$ and A, H, K as before. This proves that if $\alpha \neq 0$ then $G = 0$. Similarly, if $\beta \neq 0$ then $G = 0$.

Now suppose that $f \in \mathcal{OC}_2$ and that $\alpha = \beta = 0$ but that $e \neq 0$. Then in the same way it follows that $G = 0$.

Finally suppose that $\alpha = \beta = e = 0$, but that $G \neq 0$. Then $D = I \otimes I$ and

$$\begin{aligned}D\tfrac{1}{2}d^2 f D = {}& H \otimes I\, I \otimes S_1\, H \otimes I \\ & + I \otimes K\, S_2 \otimes I\, I \otimes K + \{H \otimes I\, S\, I \otimes K + *\} + G\{A \otimes B\, H \otimes K + *\}.\end{aligned}$$

Let $M \geq 2,\ N \geq 2$. Choose orthonormal pairs $\xi_1, \xi_2 \in \mathbb{C}^M,\ \eta_1, \eta_2 \in \mathbb{C}^N$. Let $x_1 = \xi_1 \otimes \eta_1$, $x_2 = \xi_2 \otimes \eta_2$ and $x = \varepsilon x_1 + x_2$. Choose $A,\ B,\ H,\ K$ so that

$$A\xi_2 = -\operatorname{sgn} G\delta\xi_1, \quad 0 < \|A\| = \delta < 1,$$

$$B\eta_2 = \delta\eta_1, \quad 0 < \|B\| = \delta < 1,$$

$$H\xi_1 = \xi_1,\ H\xi_2 = 0; \quad K\eta_1 = \eta_1,\ K\eta_2 = 0.$$

Then

$$\begin{aligned}&\left\langle D\tfrac{1}{2}d^2 f Dx, x\right\rangle \\ &= -2|G|\varepsilon\delta^2 + \varepsilon^2(\langle I \otimes S_1 x_1, x_1\rangle + \langle S_2 \otimes I x_1, x_1\rangle + 2\operatorname{Re}\langle S x_1, x_1\rangle + 2G\operatorname{Re}\langle A \otimes B x_1, x_1\rangle),\end{aligned}$$

which is negative if $\varepsilon > 0$ is small. This completes the proof that if $f \in \mathcal{OC}_2$ then $G = 0$.

If $M = N = 1$ then the operator function of f can be identified with f and so an operator convex function is a convex function. The proof that (1)⇒(2) is complete.

(2)⇒(3). The functions S_1, S_2 and S are continuous so that the inequalities of (3) are satisfied for all $(s,t) \in [-1,1]^2$ if and only if they are satisfied for all $(s,t) \in (-1,1)^2$. The inequalities of (3) are therefore a consequence of the elementary condition for the convexity of $f : (-1,1)^2 \to \mathbb{R}$.

(3)⇒(1). Suppose that (3) is satisfied. It will be shown that (7.14) is satisfied.

The function S_1 is a polynomial and so the set of $B \in \mathcal{S}_I(\mathbb{C}^N)$ such that $S_1(B)$ is invertible is dense in $\mathcal{S}_I(\mathbb{C}^N)$. Hence it is enough to show that condition (7.14) is satisfied by those relevant B for which $S_1(B)$ is invertible. By Thm. 7.1, if $S_1(B)$ is invertible,

$$\begin{aligned} D\tfrac{1}{2}d^2 f D &= H \otimes I\, I \otimes S_1\, D^{-1}\, H \otimes I + I \otimes K\, S_2 \otimes I\, D^{-1}\, I \otimes K \\ &\quad + \{H \otimes\, SD^{-1}\, I \otimes K + I \otimes K\, SD^{-1} H \otimes I\} \\ &= (H \otimes I\,(I \otimes S_1\, D^{-1})^{1/2} + I \otimes K\, SD^{-1}(I \otimes S_1\, D^{-1})^{-1/2}) \\ &\quad \times((I \otimes S_1\, D^{-1})^{1/2}\, H \otimes I + (I \otimes S_1\, D^{-1})^{-1/2} SD^{-1}\, I \otimes K) \\ &\quad + I \otimes K (S_2 \otimes I\, D^{-1} - SD^{-1}(I \otimes S_1\, D^{-1})^{-1} SD^{-1}) I \otimes K. \end{aligned}$$

(The operators $S_1(B)$ and $D(A,B)^{-1}$, being operator functions of (A,B), commute and are both non-negative self-adjoint.) In the latter sum the first term is the product of an operator and its adjoint and so is non-negative. It now remains to show that

$$S_2 \otimes I\, D^{-1} - S\, I \otimes S_1^{-1} SD^{-1} \geq 0,$$

which, by the commutativity of the operator functions, holds if and only if

$$S_2 \otimes S_1 - S^2 \geq 0.$$

A finite-dimensional self-adjoint operator is non-negative if and only if its eigenvalues are non-negative. The eigenvalues of $(S_2 S_1 - S^2)(A,B)$ are of the form $(S_2 S_1 - S^2)(s,t)$ where $s \in \operatorname{sp} A$ and $t \in \operatorname{sp} B$ (and similarly for $S_1(B)$ and $S_2(A)$). It therefore follows from condition (3) of the theorem that $S_1(B) \geq 0$, $S_2(A) \geq 0$ and $S_2(A) \otimes S_1(B) - S(A,B)^2 \geq 0$ for all $A \in \mathcal{S}_I(\mathbb{C}^M), B \in \mathcal{S}_I(\mathbb{C}^N)$ and all $M, N \in \mathbb{N}$. Hence condition (7.14) is satisfied.

The proof of Theorem 7.2 is complete.

8. The faces $F(\alpha,\beta,e)$ of $\mathcal{OC}_2$

In order to use the characterisation of Thm. 7.2 to investigate the faces $F(\alpha,\beta,e)$ of $\mathcal{OC}_2$ it is now necessary to calculate the second order partial derivatives of functions $f : (-1,1)^2 \to \mathbb{R}$ of the form

$$f = A + Bs + Ct + (\varDelta st + \varSigma_0 s^2 + \varGamma_0 t^2 + \varSigma_1 s^2 t + \varGamma_1 s t^2) D(s,t)^{-1}, \tag{8.1}$$

where $A, B, C, \varDelta, \varSigma_0, \varSigma_1, \varGamma_0, \varGamma_1 \in \mathbb{R}$ and the conditions

$$\varSigma_0 e + \varSigma_1 \alpha = \varGamma_0 e + \varGamma_1 \beta = 0 \tag{8.2}$$

are satisfied. For these functions one obtains, by Thm. 7.1 and elementary calculation, the following formulae:

$$(8.3)\qquad S_1 = \frac{1}{2}D^3\frac{\partial^2 f}{\partial s^2} = \Delta(\alpha - et)(1-\beta t)t + (\Sigma_0 + \Sigma_1 t)(1-\beta t)^2 + (\Gamma_0\alpha + \Gamma_1)t^2(\alpha - et).$$

One can obtain $S_2 = (1/2)D^3 f^{(0,2)}$ from (8.3) by interchanging Σ and Γ, α and β, and s and t. Next,

$$(8.4)\qquad S = \frac{1}{2}D^3\frac{\partial^2 f}{\partial s\partial t} = \Delta\left(\frac{1}{2}D + (\alpha\beta - e)st\right) + (\Sigma_0\beta + \Sigma_1)s(1-\beta t) + (\Gamma_0\alpha + \Gamma_1)t(1-\alpha s).$$

It follows in particular that $f^{(2,0)}(0,0) = 2\Sigma_0$ and $f^{(0,2)}(0,0) = 2\Gamma_0$, so that if $f \in F(\alpha,\beta,e)$ then $f \in \mathcal{K}_2$ if and only if $A = B = C = 0$ and $\Sigma_0 + \Gamma_0 = 1$.

By Thm. 7.2, the function f is operator convex if and only if

$$(8.5)\qquad S_1(t) \ge 0,\quad S_2(s) \ge 0,\quad S_1(t)S_2(s) \ge S(s,t)^2$$

for all $(s,t) \in [-1,1]^2$.

Recall that, by Prop. 6.2, equation (8.1) defines a function $f : (-1,1)^2 \to \mathbb{R}$ if and only if

$$(8.6)\qquad |\alpha+\beta| - 1 \le e \le 1 - |\alpha - \beta|$$

and then $\max\{|\alpha|,|\beta|\} \le 1$; furthermore, if $\max\{|\alpha|,|\beta|\} = 1$ then $e = \alpha\beta$.

Four questions will now be considered: (1) For which (α,β,e) are the convex cones $F(\alpha,\beta,e)$ non-trivial (i.e. $F(\alpha,\beta,e) \ne \mathcal{L}_2$ or, equivalently, $\dim F(\alpha,\beta,e) > 3$)? (2) What is the intersection of two distinct members of the family? (3) What is the dimension of $F(\alpha,\beta,e)$? (4) What is the set of extreme points of the set $F(\alpha,\beta,e)\cap\mathcal{K}_2$? The authors' present state of knowledge will be presented in four composite theorems. The analysis is elementary, sometimes lengthy but surprisingly calculable. Some details and some proofs will be omitted.

Theorem 8.1. (1) *$\{e : F(\alpha,\beta,e) \ne \mathcal{L}_2\}$ is a closed subset of the interval $[|\alpha+\beta|-1, 1-|\alpha-\beta|]$. Let e_{m} and e_{M} denote the minimum and maximum of $\{e : F(\alpha,\beta,e) \ne \mathcal{L}_2\}$ when the set is non-empty.*

(2) *Suppose $F(\alpha,\beta,e) \ne \mathcal{L}_2$. Then $|e| \le \min\{|\alpha|,|\beta|\}$. If $|e| = \min\{|\alpha|,|\beta|\}$ then $e = \alpha\beta$ and either $\alpha\beta = 0$ or $\max\{|\alpha|,|\beta|\} = 1$.*

(3) *If $\alpha\beta > 0$ and $\max\{|\alpha|,|\beta|\} < 1$ then*

$$(8.7)\qquad \alpha\beta < e_{\mathrm{M}} < \min\{|\alpha|,|\beta|\} < 1 - |\alpha-\beta|$$

and

$$(8.8)\qquad |\alpha+\beta| - 1 = e_{\mathrm{m}} \quad \text{if } |\alpha+\beta| \ge 1,$$

$$(8.9)\qquad |\alpha+\beta| - 1 < e_{\mathrm{m}} \quad \text{if } |\alpha+\beta| < 1.$$

There is a corresponding statement for $\alpha\beta < 0$.

(It is not known whether $\{e : F(\alpha,\beta,e) \ne \mathcal{L}_2\}$ must be either empty or an interval.)

THEOREM 8.2. *If* $(\alpha,\beta,e)\neq(\alpha',\beta',e')$ *and* $F(\alpha,\beta,e)\cap F(\alpha',\beta',e')\cap\mathcal{K}_2$ *is non-empty then* $e=\alpha\beta$, $e'=\alpha'\beta'$ *and either* $\beta=\beta'$ *and the intersection is* $\{t^2(1-\beta t)^{-1}\}$, *or* $\alpha=\alpha'$ *and the intersection is* $\{s^2(1-\alpha s)^{-1}\}$. *Consequently, the functions* $t^2(1-\beta t)^{-1}$ *and* $s^2(1-\alpha s)^{-1}$ *are extreme points of* $\mathcal{K}_2$.

The proof of Theorem 8.2 is omitted.

THEOREM 8.3. (1) *Suppose* $\alpha\beta\neq 0$, *and* $\max\{|\alpha|,|\beta|\}<1$.

(a) *For each* e, *the convex cone* $F(\alpha,\beta,e)$ *has dimension* 3 (*the trivial case*), 4 *or* 6.

(b) $\{e:\dim F(\alpha,\beta,e)=6\}$ *is a relatively open subset of the interval* $[|\alpha+\beta|-1, 1-|\alpha-\beta|]$ *and contains* $\alpha\beta[0,1]\cap[|\alpha+\beta|-1,1-|\alpha-\beta|]$.

If $\alpha\beta>0$ *then* $\dim F(\alpha,\beta,e_{\mathrm{M}})=4$.

If $\alpha\beta>0$ *and* $|\alpha+\beta|<1$ *then* $\dim F(\alpha,\beta,e_{\mathrm{m}})=4$.

There are corresponding statements for $\alpha\beta<0$.

(2) *If* $\alpha\beta\neq 0$ *then* $\dim F(\alpha,\beta,\alpha\beta)=6$ *and the function* $(1-\alpha s)^{-1}(1-\beta t)^{-1}$ *is in the relative interior of* $F(\alpha,\beta,\alpha\beta)$.

(3) *If* $\alpha\neq 0$ *then* $\dim F(\alpha,0,0)=7$.

(4) $\dim F(0,0,0)=8$.

It is not known whether the sets $\{e:\dim F(\alpha,\beta,e)=4\}$ can contain points other than those identified in (1).

THEOREM 8.4. *If* $\alpha\beta\neq 0$, $\max\{|\alpha|,|\beta|\}<1$ *and* $|\alpha+\beta|-1<e<1-|\alpha-\beta|$ *then each point of the relative boundary of the convex set* $F(\alpha,\beta,e)\cap\mathcal{K}_2$ *is an extreme point of* $\mathcal{K}_2$.

The authors' further analysis of the extreme point sets of $F(\alpha,\beta,e)\cap\mathcal{K}_2$ is lengthy, though incomplete, and at present of insufficient interest to merit inclusion in this paper. We only mention that in Cases (2) ($\max\{\alpha,\beta\}=1$), (3) and (4) below, the relative boundary of $F(\alpha,\beta,e)\cap\mathcal{K}_2$ contains non-degenerate line segments.

The rest of this section discusses the proofs of Theorems 8.1–8.4. Additional theorems are technical in nature.

THEOREM 8.5. *If* $(\alpha,\beta,e)\in\mathbb{R}^3$, $F(\alpha,\beta,e)\neq\mathcal{L}_2$, *a function* f *given by* (8.1) *is in* $F(\alpha,\beta,e)\setminus\mathcal{L}_2$ *and* $S_1(t_0)=0$ *for some* $t_0\in[-1,1]$, *then* $e\in\alpha\beta[0,1]$.

PROOF. By Prop. 6.2, if $1-\beta t_0=0$ then $|\beta|=1$ and $e=\alpha\beta$, so the conclusion is satisfied.

Suppose $1-\beta t_0\neq 0$. By condition (8.5), $S(s,t_0)=0$ for all $s\in[-1,1]$ from which it follows that

$$\varDelta=\frac{-2(\varGamma_0\alpha+\varGamma_1)t_0}{1-\beta t_0}, \tag{8.10}$$

$$\varSigma_0\beta+\varSigma_1=\frac{(\varGamma_0\alpha+\varGamma_1)t_0^2(\alpha\beta-e)}{(1-\beta t_0)^2}.$$

Substituting for $\varDelta$ in the expression for $S_1(t_0)=0$ we deduce that

$$\varSigma_0+\varSigma_1 t_0=\frac{(\varGamma_0\alpha+\varGamma_1)t_0^2(\alpha-e t_0)}{(1-\beta t_0)^2}.$$

From the latter two equations one finds that

$$\Sigma_0 = \frac{(\Gamma_0\alpha + \Gamma_1)t_0^2\alpha}{(1-\beta t_0)^2}, \tag{8.11}$$

$$\Sigma_1 = \frac{(\Gamma_0\alpha + \Gamma_1)t_0^2(-e)}{(1-\beta t_0)^2} \tag{8.12}$$

and

$$\Sigma_0 + \Sigma_1 t = \frac{(\Gamma_0\alpha + \Gamma_1)t_0^2(\alpha - et)}{(1-\beta t_0)^2}.$$

Substituting for Δ and $\Sigma_0 + \Sigma_1 t$ in the formula for S_1 we obtain

$$S_1(t) = \frac{(\Gamma_0\alpha + \Gamma_1)(t-t_0)^2(\alpha - et)}{(1-\beta t_0)^2}.$$

Substituting for Δ and $\Sigma_0\beta + \Sigma_1$ in the formula for S_2, and using the relation

$$(\Gamma_0\alpha + \Gamma_1)(\beta - es) = (\Gamma_0 + \Gamma_1 s)(\alpha\beta - e)$$

(a consequence of (8.2)), we obtain

$$S_2(s) = \frac{(\Gamma_0 + \Gamma_1 s)D(s,t_0)^2}{(1-\beta t_0)^2}.$$

Similarly,

$$S(s,t) = \frac{(\Gamma_0\alpha + \Gamma_1)D(s,t_0)(t-t_0)}{(1-\beta t_0)^2}.$$

Therefore, for all $(s,t) \in [-1,1]^2$,

$$0 \le S_1(t)S_2(s) - S(s,t)^2 = -(\Gamma_0\alpha + \Gamma_1)\Gamma_1 D(s,t_0)^2 D(s,t)\frac{(t-t_0)^2}{(1-\beta t_0)^4}.$$

The condition $1 - \beta t_0 \neq 0$ entails that $D(s,t_0) \neq 0$ for some $s \in [-1,1]$. Consequently,

$$0 \le -(\Gamma_0\alpha + \Gamma_1)\Gamma_1.$$

If $\Gamma_0\alpha$ were zero then it would follow that $\Gamma_1 = 0$ and then, by (8.10), (8.11), and (8.12), that $f \in \mathcal{L}_2$, which is a contradiction. So $\Gamma_0 \neq 0$ and, by (8.2),

$$0 \le -(\Gamma_0\alpha + \Gamma_1)\Gamma_1\beta^2 = \Gamma_0^2(\alpha\beta - e)e$$

and therefore $e \in \alpha\beta[0,1]$.

Proof of Theorem 8.1(1), (2). For (1) notice that the functions S_1, S_2 and S are continuous functions of all the variables. The assertion is given by a simple compactness argument.

(2) Now suppose that $f \in F(\alpha,\beta,e) \setminus \mathcal{L}_2$ and that $0 \neq |e| \ge |\alpha|$. Then $\Sigma_0 + \Sigma_1 t = \Sigma_1(\alpha - et)/e$, α/e is a zero of S_1 and $\alpha/e \in [-1,1]$. Therefore $e \in \alpha\beta[0,1]$ by Thm. 8.5. The statement (2) now follows.

The four cases of Thm. 8.3 require separate discussion. In Cases (1) and (2) one can substitute $\Sigma_1 = -e\Sigma_0/\alpha$, $\Gamma_1 = -e\Gamma_0/\beta$ and regard S_1, S_2 and S as linear functions of $\pi = (\Delta, \Sigma_0, \Gamma_0) \in \mathbb{R}^3$. In Cases (2)–(4) condition (8.5) for the convexity of the function f of (8.1) can be simplified. We introduce a notation which is common to the four cases, but first we state a simple proposition.

PROPOSITION 8.6. *Let* $C = \{(x, y, z) \in \mathbb{R}^3 : x \geq 0,\ y \geq 0,\ xy = z^2\}$. *Then* C *is a closed convex cone and each boundary ray of* C *is an extremal subset of* C.

The four cases are now described.

CASE (1): $\alpha\beta \neq 0,\ \max\{|\alpha|, |\beta|\} < 1$. Let $d_1 = 3$. For $\pi = (\Delta, \Sigma_0, \Gamma_0) \in \mathbb{R}^3 = \mathbb{R}^{d_1}$ let

$$f_\pi = \left(\Delta st + \Sigma_0 s^2\left(1 - \frac{e}{\alpha}t\right) + \Gamma_0 t^2\left(1 - \frac{e}{\beta}s\right)\right)D(s,t)^{-1} \tag{8.13}$$

and write

$$T_1(\pi; t) = S_1(\pi; t) = \frac{\alpha - et}{\alpha}\left(\Delta\alpha(1-\beta t)t + \Sigma_0(1-\beta t)^2 + \Gamma_0\frac{\alpha}{\beta}(\alpha\beta - e)t^2\right), \tag{8.14}$$

$T_2(\pi; s) = S_2(\pi; s)$ for the corresponding expression for $\frac{1}{2}D^2 f_\pi^{(0,2)}$ and

$$\begin{aligned} T(\pi; s, t) = S(\pi, s, t) = \Delta\left(\frac{1}{2}D(s,t) + (\alpha\beta - e)st\right) \\ + \Sigma_0\frac{\alpha\beta - e}{\alpha}s(1-\beta t) + \Gamma_0\frac{\alpha\beta - e}{\beta}t(1-\alpha s). \end{aligned} \tag{8.15}$$

Define $\Phi_{s,t}^{(1)} : \mathbb{R}^3 \to \mathbb{R}^3$ by

$$\Phi_{s,t}^{(j)}(\pi) = (T_1(\pi; t), T_2(\pi; s), T(\pi; s, t)) \tag{8.16}$$

with $j = 1$ on the left. In Cases (2)–(4) below the mappings $\Phi_{s,t}^{(j)}$ for $j = 2, 3, 4$ are defined in the same way.

CASE (2): $e = \alpha\beta \neq 0$. Note that this case overlaps Case (1), though the principal concern here is when $\max\{|\alpha|, |\beta|\} = 1$.

In this case $D(s,t) = (1 - \alpha s)(1 - \beta t)$.

Let $d_2 = 3$. For $\pi = (\Delta, \Sigma_0, \Gamma_0) \in \mathbb{R}^3 = \mathbb{R}^{d_2}$ the equation (8.13) now becomes

$$f_\pi = \Delta st(1-\alpha s)^{-1}(1-\beta t)^{-1} + \Sigma_0 s^2(1-\alpha s)^{-1} + \Gamma_0 t^2(1-\beta t)^{-1}. \tag{8.17}$$

Let

$$\begin{aligned} T_1(\pi; t) &= \Delta\alpha t + \Sigma_0(1-\beta t), \quad \text{so that} \quad S_1(\pi; t) = (1-\beta t)^2 T_1(\pi; t), \\ T_2(\pi; s) &= \Delta\beta s + \Gamma_0(1-\alpha s), \quad \text{so that} \quad S_2(\pi; s) = (1-\alpha s)^2 T_2(\pi; s), \\ T(\pi; s, t) &= \tfrac{1}{2}\Delta, \quad \text{so that} \quad S(\pi; s, t) = (1-\alpha s)(1-\beta t)T(\pi; s, t). \end{aligned}$$

CASE (3): $\alpha \neq 0, e = \beta = 0$. Let $d_3 = 4$. For $\pi = (\Delta, \Sigma_0, \Gamma_0, \Gamma_1) \in \mathbb{R}^4 = \mathbb{R}^{d_3}$ write

$$f_\pi = (\Delta st + \Sigma_0 s^2 + \Gamma_0 t^2 + \Gamma_1 st^2)(1-\alpha s)^{-1}. \tag{8.18}$$

(The right hand side is obtained from the right hand side of (8.1) by putting $A = B = C = 0$ and substituting $\Sigma_1 = -e\Sigma_0/\alpha = 0$.)

Let

$$T_1(\pi; t) = S_1(\pi, t) = \Delta\alpha t + \Sigma_0 + (\Gamma_0\alpha + \Gamma_1)\alpha t^2.$$

Next let

$$T_2(\pi;s) = \Gamma_0 + \Gamma_1 s \quad \text{so that} \quad S_2(\pi;s) = (1-\alpha s)^2 T_2(\pi;s),$$
$$T(\pi;s,t) = \Delta/2 + (\Gamma_0\alpha + \Gamma_1)t \quad \text{so that} \quad S(\pi;s,t) = (1-\alpha s)T(\pi;s,t).$$

CASE (4): $(\alpha,\beta,e) = (0,0,0)$. Let $d_4 = 5$. For $\pi = (\Delta,\Sigma_0,\Gamma_0,\Sigma_1,\Gamma_1) \in \mathbb{R}^5 = \mathbb{R}^{d_4}$ write

$$f_\pi = \Delta st + \Sigma_0 s^2 + \Gamma_0 t^2 + \Sigma_1 s^2 t + \Gamma_1 t^2 s$$

and let

$$T_1(\pi;t) = S_1(\pi;t) = \Sigma_0 + \Sigma_1 t,$$
$$T_2(\pi;s) = S_2(\pi;s) = \Gamma_0 + \Gamma_1 s,$$
$$T(\pi;s,t) = S(\pi;s,t) = \tfrac{1}{2}\Delta + \Sigma_1 s + \Gamma_1 t.$$

Now let j be any one of 1, 2, 3 and 4. If $\pi \in \mathbb{R}^{d_j}$ then the condition (8.5) for f_π to be convex and operator convex reduces to:

(8.19) $$T_1(\pi;t) \geq 0, \quad T_2(\pi;s) \geq 0, \quad (T_1T_2 - T^2)(\pi;s,t) \geq 0$$

for all $(s,t) \in [-1,1]^2$.

If (α,β,e) belongs to Case (j) let

$$\Pi^{(j)} = \{\pi \in \mathbb{R}^{d_j} : f_\pi \in F(\alpha,\beta,e)\}.$$

Note that

$$F(\alpha,\beta,e) = \mathcal{L}_2 + \{f_\pi : \pi \in \Pi^{(j)}\},$$
$$\dim F(\alpha,\beta,e) = 3 + \dim \Pi^{(j)},$$
$$F(\alpha,\beta,e) \cap \mathcal{K}_2 = \{f_\pi : \pi \in \Pi^{(j)}, \Sigma_0 + \Gamma_0 = 1\}.$$

Condition (8.19) can now be expressed in the form

(8.20) $$\Pi^{(j)} = \bigcap_{(s,t)\in[-1,1]^2} \Phi_{s,t}^{(j)\,-1}(C).$$

Information about the mappings $\Phi_{s,t}^{(j)}$, $j = 1,2,3,4$, is given by the next lemma. The next two lemmas are primarily concerned with formulae for which there exist pedestrian verifications.

In Lemma 8.8 it will only be assumed that $\alpha\beta \neq 0$ (Case (1) or Case (2)) and S_1, S_2 and S will be regarded as functions of $\pi = (\Delta,\Sigma_0,\Gamma_0) \in \mathbb{R}^3$, as in Case (1). For $\pi = (\Delta,\Sigma_0,\Gamma_0)$ we will write

$$\theta_{s,t}(\pi) = \Delta st + \frac{\Sigma_0}{\alpha}s(1-\beta t) + \frac{\Gamma_0}{\beta}t(1-\alpha s).$$

LEMMA 8.7. (1) *Suppose that $\alpha\beta \neq 0$. Then*

(8.21) $$\det \Phi_{s,t}^{(1)} = \frac{(\alpha - et)(\beta - es)}{2\alpha\beta} D(s,t)^3.$$

If $(s,t) \in [-1,1]^2$ then $\det \Phi_{s,t}^{(1)} = 0$ if and only if either

(i) $\max\{|\alpha|,|\beta|\} = 1$, $e = \alpha\beta$ *and* $(1-\alpha s)(1-\beta t) = 0$, *or*

(ii) $\max\{|\alpha|,|\beta|\} < 1$, $D(s,t) = 0$, *either* $e = |\alpha+\beta| - 1$ *or* $e = 1 - |\alpha-\beta|$ *and* $|s| = |t| = 1$. (*Compare Thm.* 8.1(3).)

If $|s| = |t| = 1$, $D(s,t) = 0$, *and* $\pi = (\Delta, \Sigma_0, \Gamma_0)$ *then*

$$\Phi^{(1)}_{s,t}(\pi) = \theta_{s,t}(\pi)((1-\beta t)^2, (1-\alpha s)^2, (1-\alpha s)(1-\beta t)st). \tag{8.22}$$

(2) *The mappings* $\Phi^{(3)}_{s,t} : \mathbb{R}^4 \to \mathbb{R}^3$ *and* $\Phi^{(4)}_{s,t} : \mathbb{R}^5 \to \mathbb{R}^3$ *are surjective for each* $(s,t) \in [-1,1]^2$.

Lemma 8.8. *Suppose* $\alpha\beta \neq 0$, $\pi = (\Delta, \Sigma_0, \Gamma_0) \in \mathbb{R}^3$. *Then*

$$\begin{aligned}(S_1S_2 - S^2)(\pi; s,t) \\ &= D\bigg(e(\alpha\beta - e)\theta_{s,t}(\pi)^2 + \Delta e D\theta_{s,t}(\pi) + D\bigg(\frac{\Sigma_0}{\alpha}\frac{\Gamma_0}{\beta}(\alpha\beta - e + eD) - \frac{\Delta^2}{4}\bigg)\bigg).\end{aligned}$$

(*Note that* $\alpha\beta - e + eD = (\alpha - et)(\beta - es)$.)

The next theorem is the key to the analysis of the facial structure of the convex cones $F(\alpha,\beta,e)$. In particular, Thm. 8.4 is an immediate consequence of part (3) of the theorem.

Theorem 8.9. *Suppose* (α,β,e) *belongs to Case* (j) *for* $j = 1,2,3$ *or* 4.

(1) *If* $\pi \in \mathbb{R}^{d_j}$ *and* $\Phi^{(j)}_{s,t}(\pi) \in \operatorname{int} C$ *for all* $(s,t) \in [-1,1]^2$ *then* $\pi \in \operatorname{int} \Pi^{(j)}$ *and* $\dim \Pi^{(j)} = d_j$.

(2) *Suppose* $\pi \in \Pi^{(j)}$ *and let* E_π *be the minimal extremal subset of* $\Pi^{(j)}$ *containing* π. *If* $(s,t) \in [-1,1]^2$, *the mapping* $\Phi^{(j)}_{s,t} : \mathbb{R}^{d_j} \to \mathbb{R}^3$ *is surjective*, $\mathbf{x} = \Phi^{(j)}_{s,t}(\pi) \in \operatorname{bdy} C$, H_π *is a support hyperplane to* C *at* $\mathbf{x}$ (*unique if* $\mathbf{x} \neq 0$), *then* $\pi \in \operatorname{bdy} \Pi^{(j)}$ *and* $E_\pi \subseteq \Phi^{(j)\,-1}_{s,t}(H_\pi) \cap \Pi^{(j)}$.

(3) *If* (α,β,e) *belongs to Case* (1) *and* $|\alpha+\beta| - 1 < e < 1 - |\alpha-\beta|$ *then* $\dim \Pi^{(1)}$ *is* 0, 1, *or* 3. *If* $\dim \Pi^{(1)} = 3$ *then each boundary ray of* $\Pi^{(1)}$ *is an extremal and exposed subset of* $\Pi^{(1)}$.

(4) *Suppose that* $j = 2$ *or* 3 *and that* $\dim \Pi^{(j)} = d_j$. *If* $\pi \in \Pi^{(j)}$ *then* $\pi \in \operatorname{bdy} \Pi^{(j)}$ *if and only if* $\Phi^{(j)}_{s,t}(\pi) \in \operatorname{bdy} C$ *for some* $(s,t) \in [-1,1]^2$. *If* (s,t) *satisfies this condition and* H_π *is a support hyperplane to* C *at* $\Phi^{(j)}_{s,t}(\pi)$ *then* $\Phi^{(j)-1}_{s,t}(H_\pi) \cap \Pi^{(j)}$ *is a face of* $\Pi^{(j)}$ *which contains* E_π. *Every maximal face of* $\Pi^{(j)}$ *is of this form.*

Proof. (1) The hypothesis of (1) is equivalent to the inequalities of (8.19) being strict for each $(s,t) \in [-1,1]^2$. The functions T_1, T_2 and T are continuous functions of π and (s,t) and so the inequalities remain strict after small perturbations of π. This proves (1). It follows that if $\pi \in \operatorname{bdy} \Pi^{(j)}$ then $\Phi^{(j)}_{s,t}(\pi) \in \operatorname{bdy} C$ for some $(s,t) \in [-1,1]^2$.

(2) Let H_π be the null space of a linear functional $\mathbf{x}^*$ on $\mathbb{R}^3$. Then, since $\Phi^{(j)}_{s,t}$ is surjective, $\mathbf{x}^*\Phi^{(j)}_{s,t}$ is a non-zero linear functional on $\mathbb{R}^{d_j}$ and its null space $\Phi^{(j)\,-1}_{s,t}(H_\pi)$ is a hyperplane in $\mathbb{R}^{d_j}$ and $\Pi^{(j)}$ is contained in one of its closed half-spaces. The set E_π is the union of those line segments in $\Pi^{(j)}$ which pass through π and $\pi \in \Phi^{(j)\,-1}_{s,t}(H_\pi)$. Therefore $E_\pi \subseteq \Phi^{(j)\,-1}_{s,t}(H_\pi) \cap \Pi^{(j)}$.

(3) By Lemma 8.7 and the hypothesis of (3) the mapping $\Phi^{(1)}_{s,t}$ is bijective for each $(s,t) \in [-1,1]^2$. Suppose $\pi \in \operatorname{bdy} \Pi^{(1)}$ and (s,t) is such that $\Phi^{(1)}_{s,t}(\pi) \in \operatorname{bdy} C$ (there is

such by (1)). Then, by (2) and Prop. 8.6,

$$\mathbb{R}^+\pi \subseteq E_\pi \subseteq \Phi_{s,t}^{(1)\,-1}(H_\pi) \cap \Pi^{(1)} \subseteq \Phi_{s,t}^{(1)\,-1}(\mathbb{R}\Phi_{s,t}^{(1)}(\pi)) \cap \Pi^{(1)} = \mathbb{R}^+\pi.$$

If $\dim \Pi^{(1)} < 3$ and $\pi \in \operatorname{relint} \Pi^{(1)}$ then $\pi \in \operatorname{bdy} \Pi^{(j)}$ and $E_\pi = \Pi^{(1)}$.

(4) By Lemma 8.7 the mappings $\Phi_{s,t}^{(3)}$ and $\Phi_{s,t}^{(4)}$ are surjective for each $(s,t) \in [-1,1]^2$. Suppose that π, (s,t) and H_π are as stated, and so as in (2). Then by (2), $\Phi_{s,t}^{(j)-1}(H_\pi)$ is a support hyperplane to $\Pi^{(j)}$ at π so that the first conclusion of (4) holds. If E is a maximal face of $\Pi^{(j)}$ and $\pi \in \operatorname{relint} E$ then it follows that $E = E_\pi = \Phi_{s,t}^{(j)\,-1}(H_\pi) \cap \Pi^{(j)}$.

The proofs of Theorems 8.1 and 8.3 can now be completed.

Case (1). One may restrict attention to the first quadrant of the (α,β)-plane. Results for the other quadrants can then be obtained by means of the reflections $s \mapsto -s$ and $t \mapsto -t$. So, suppose that $0 < \alpha < 1,\ 0 < \beta < 1$.

Then $\min\{\alpha,\beta\} < 1 - |\alpha - \beta|$ and, by Thm. 8.1, $e_{\mathrm{M}} < \min\{\alpha,\beta\}$. Thus two of the inequalities of (8.7) hold. If $\alpha + \beta - 1 < e \le e_{\mathrm{M}}$ then, by Thm. 8.9(3), $\dim F(\alpha,\beta,e) = 3 + \dim \Pi^{(1)} = 3, 4,$ or 6.

Suppose that $\alpha + \beta - 1 = e$ and $F(\alpha,\beta,e) \ne \mathcal{L}_2$. Then $D(s,t) = 0$ if and only if $(s,t) = (1,1)$, so, by Thm. 8.1(2) and Lemma 8.7(1), $\det \Phi_{s,t}^{(1)} = 0$ if and only if $s = t = 1$. By (8.22) of Lemma 8.7(1),

$$(S_1S_2 - S^2)(\pi;1,1) = 0 \tag{8.23}$$

for all $\pi \in \mathbb{R}^3$. Now one calculates that

$$\frac{\partial}{\partial t}(S_1S_2 - S^2)(\pi;1,1) = -e\theta_{1,1}(\pi)^2(1-\alpha)^2(1-\beta). \tag{8.24}$$

If $\pi \in F(\alpha,\beta,e) \setminus \mathcal{L}_2$ then condition (8.5) requires that $\frac{\partial}{\partial t}(S_1S_2 - S^2)(\pi;1,1) \le 0$, so that either $\theta_{1,1}(\pi) = 0$ or $e \ge 0$. However, if $\theta_{1,1}(\pi) = 0$ then $S_1(\pi,1) = 0$ by (8.22) and so $e \in \alpha\beta[0,1]$ by Thm. 8.5. This proves that $\alpha + \beta \ge 1$. The assertion (8.9) of Thm. 8.1(3) follows.

Now suppose further that $e = \alpha + \beta - 1 > 0$ and $\pi = (0, \Sigma_0, \Gamma_0)$ where $\Sigma_0 > 0,\ \Gamma_0 > 0$. Then $S_1(\pi,t) > 0$ and $S_2(\pi,s) > 0$ for all $s,t \in [-1,1]$ and, by Lemma 8.8, $(S_1S_2 - S^2)(\pi;s,t) > 0$ for all $(s,t) \ne (1,1)$. Also, by (8.24) (and its companion)

$$\frac{\partial}{\partial t}(S_1S_2 - S^2)(\pi;1,1) < 0, \quad \frac{\partial}{\partial s}(S_1S_2 - S^2)(\pi;1,1) < 0. \tag{8.25}$$

The inequalities (8.25) continue to hold after small perturbations of π so there exists an open neighbourhood N of $(1,1)$ in $[-1,1]^2$ and a neighbourhood W of π in $\mathbb{R}^3$ such that $(S_1S_2 - S^2)(\pi';s,t) \ge 0$ for all $(\pi';s,t) \in W \times N$. Then there exists a neighbourhood W' of π such that $(S_1S_2 - S^2)(\pi';s,t) \ge 0$ for all $(\pi';s,t) \in W' \times ([-1,1]^2 \setminus N)$. This proves that $\pi \in \operatorname{int} \Pi^{(1)}$ and $\dim F(\alpha,\beta,\alpha+\beta-1) = 6$.

If $e = \alpha + \beta - 1 = 0$ then $(0,\Sigma_0,\Gamma_0) \in \Pi^{(1)}$ if $\Sigma_0 \ge 0,\ \Gamma_0 \ge 0$; one also verifies that $(\alpha s + \beta t)^2(1 - \alpha s - \beta t)^{-1} \in F(\alpha,\beta,0)$ so that again $\dim F(\alpha,\beta,0) = 6$.

Thus if $0 < \alpha < 1,\ 0 < \beta < 1$ and $e = \alpha + \beta - 1 \ge 0$ then $\dim F(\alpha,\beta,0) = 6$. Hence (8.8) of Thm. 8.1(3) is established.

Now suppose that $0 < \alpha < 1,\ 0 < \beta < 1$, that $e \in \alpha\beta[0,1]$ and $\alpha + \beta - 1 < e$. If $\pi = (0, \Sigma_0, \Gamma_0)$, where $\Sigma_0 \geq 0,\ \Gamma_0 \geq 0$, then, by Lemma 8.8, $\pi \in \Pi^{(1)}$. Thus $\dim F(\alpha, \beta, e) \geq 2$ and so, by Thm. 8.9(3), is $= 3$.

Suppose that $0 < \alpha < 1,\ 0 < \beta < 1$ and $\alpha + \beta - 1 < e \leq e_{\mathrm{M}}$. If $\dim \Pi^{(1)} = 3$ and $\pi \in \operatorname{int} \Pi^{(1)}$ then, by Lemma 8.7(1), $\det \Phi^{(1)}_{s,t} \neq 0$ for all $(s,t) \in [-1,1]^2$ and, by Thm. 8.9(2), $\Phi^{(1)}_{s,t}(\pi) \in \operatorname{int} C$ for all $(s,t) \in [-1,1]^2$, which is to say that the inequalities in (8.5) are all strict. They remain strict under small perturbations of e. Part (1)(b) of Thm. 8.3 now follows, by using Thm. 8.9. The first inequality of (8.7) also follows.

Case (2). Suppose $e = \alpha\beta \neq 0$,

$$\frac{1}{(1-\alpha s)(1-\beta t)} = 1 + \alpha s + \beta t + f_\pi(s,t)$$

where $\pi = (\alpha\beta, \alpha^2, \beta^2)$. Then $\Phi^{(2)}_{s,t}(\pi) = \left(\alpha^2, \beta^2, \frac{1}{2}\alpha\beta\right)$ and the conditions (8.19) are satisfied with strict inequalities. Part (2) of Thm. 8.3 now follows from Thm. 8.9(1).

Case (3) and Case (4). The proofs of (3) and (4) of Thm. 8.3 follow that of (2). If $\Sigma_0 > 0$ and $\Gamma_0 > 0$ then $(0, \Sigma_0, \Gamma_0, 0) \in \operatorname{int} \Pi^{(3)}$. If $\Sigma_0 > 0,\ \Gamma_0 > 0$ and $4\Sigma_0\Gamma_0 > \Delta^2$ then $\pi = (\Delta, \Sigma_0, \Gamma_0, 0, 0) \in \operatorname{int} \Pi^{(4)}$.

The proofs are now complete.

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