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Convexity and Concavity of Eigenvalue Sums

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It is well known that $\sigma(H)$, the sum of the negative eigenvalues of a Hermitian matrix H, is a concave and increasing function of H. In contrast to this, we prove that for A nonsingular Hermitian and P positive definite, the function $P \mapsto \sigma(AP) = \sigma(P^{1/2}AP^{1/2})$ is convex and decreasing. Several other results of this nature are also proved.

KEY WORDS: Convexity; concavity; eigenvalues.

Eigenvalue inequalities play an important role in quantum mechanics. A person who contributed much to the development of this subject was Jerome Percus, and it is with this thought in mind that we dedicate this article to him on the occasion of his 65th birthday.

A quantum mechanical Hamiltonian or density matrix is an $N \times N$ Hermitian matrix (we deal here with the finite-dimensional case for simplicity) and we shall denote such a matrix generically by H. It is well known that the sum of the lowest n eigenvalues of H (for any $n \geqslant 1$), as well as $\sigma(H)$, the sum of all the negative eigenvalues of H, are concave functions of H. These facts follow easily from the variational principle. Examples of their usefulness include the theory of crystallization in the Falicov–Kimball (or static) model,(1) the monotonicity of electronic energies with respect to molecular displacement,(2) the theory of molecular binding,[3] and the theory of density matrices and their mixing properties.(6,7) In general, if H is a "one-particle Hamiltonian," then $-2\sigma(H)$ is

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the maximum binding energy of spin-1/2 fermions, whence the importance of $\sigma(H)$ for the quantum mechanical many-body problem.

It was with some surprise, therefore, that we discovered that a seemingly similar eigenvalue problem changes concavity into convexity. Instead of $\sigma(H)$ for H Hermitian, we investigated $\sigma(AP)$, where A is some *fixed* Hermitian matrix with n negative and $N-n$ positive eigenvalues, and P is an arbitrary positive-definite matrix. [Since spectrum$(AP)=$ spectrum$(P^{1/2}AP^{1/2})$, the eigenvalues of AP are all real.] As a function of P, the sum of the negative eigenvalues $\sigma(AP)$ is convex! This conclusion also has generalizations that will be given later. Since there are so few general theorems available about the dependence of eigenvalues on adjustable parameters, we present our result in the hope that it may eventually be of use in quantum mechanics. Actually, we discovered it in connection with our investigation of the Scott conjecture for molecules.

The $\sigma(AP)$ problem may seem artificial compared to the $\sigma(H)$ problem, but actually they are closely related. Suppose $\mathscr{H}$ is a Hilbert space with inner product $\langle \cdot, \cdot \rangle$ and that we consider a finite-rank, self-adjoint linear operator H whose action on a vector f is given in the form

$$Hf = \sum_{i=1}^{N} \varepsilon_i \langle g_i, f \rangle g_i \tag{1}$$

where the g_i are N linearly independent vectors in $\mathscr{H}$ and $\varepsilon_i = -1$ for $i = 1,..., n$ and $\varepsilon_i = +1$ for $i = n+1,..., N$. The operator H in the form (1) can easily arise as an approximation (or a bound) to some given Hamiltonian of interest. If the g_i are *not* orthogonal to each other, the computation of the eigenvalues of H may not be trivial. The simplest way to compute them is to write an eigenvector f in the subspace spanned by the g_i as

$$f = \sum_{i=1}^{N} v_i g_i \tag{2}$$

and then use the linear independence of the g_i to conclude that $Hf = \lambda f$ is equivalent to

$$APV = \lambda V \tag{3}$$

with $V = (v_1,..., v_N)$, $A = \operatorname{diag}(\varepsilon_1,..., \varepsilon_N)$, and $P_{ij} = \langle g_i, g_j \rangle$. Thus, while the nonzero eigenvalues of H and of AP are identical, the quantity $\sigma(H) = \sigma(AP)$ will be seen to be concave in H, but convex in P!

Before stating our results formally, let us first state some definitions and well-known facts. We set

$$\mathscr{H}_N = \{\text{Hermitian } N \times N \text{ matrices}\}$$

$$\mathscr{P}_N = \{\text{positive-definite matrices} \in \mathscr{H}_N\}$$

$$\lambda_1(H) \leqslant \lambda_2(H) \leqslant \cdots \leqslant \lambda_N(H) \text{ are the eigenvalues of } H \in \mathscr{H}_N \tag{4}$$

For $1 \leqslant k \leqslant N$ we define

$$\sigma_{(k)}(H) \equiv \sum_{j=1}^{k} \lambda_j(H) \tag{5}$$

$$\sigma^{(k)}(H) \equiv \sum_{j=N-k+1}^{N} \lambda_j(H) = \text{Trace } H - \sigma_{(k)}(H) \tag{6}$$

For $c \in \mathbf{R}$ we define

$$\sigma_c(H) \equiv \sum_{j=1}^{N} \min\{\lambda_j(H) - c, 0\} \tag{7}$$

$$\sigma^c(H) \equiv \sum_{j=1}^{N} \max\{\lambda_j(H) - c, 0\} = \text{Trace } H - cN - \sigma_c(H) \tag{8}$$

In particular, $\sigma(H) = \sigma_0(H)$.

The following, (9)–(13), are well-known easy consequences of the min-max principle (for example). They are listed here for comparison with our AP results in the theorem below:

$$H \mapsto \sigma_{(k)}(H) \text{ is concave and increasing} \tag{9}$$

$$H \mapsto \sigma^{(k)}(H) \text{ is convex and increasing} \tag{10}$$

$$H \mapsto \sigma_c(H) \text{ is concave and increasing} \tag{11}$$

$$H \mapsto \sigma^c(H) \text{ is convex and increasing} \tag{12}$$

$$H \mapsto \lambda_j(H) \text{ is increasing for each } j \tag{13}$$

{Here, $H \mapsto f(H)$ is concave means $f(sH + (1-s)B) \geqslant sf(H) + (1-s)f(B)$, while $f(H)$ is convex means $-f(H)$ is concave. $H \mapsto f(H)$ is increasing (resp. decreasing) means $B - H \in \mathscr{P}_N$ implies $f(B) \geqslant f(H)$ [resp. $f(B) \leqslant f(H)$].}

Now let us fix N and some *nonsingular* $A \in \mathscr{H}_N$. Let $n \in \{0, \ldots, N\}$ be the number of negative eigenvalues of A (whence A has $N - n$ positive eigenvalues). For each $P \in \mathscr{P}_N$, the eigenvalues of AP are identical to those of $P^{1/2}AP^{1/2} \in \mathscr{H}_N$ and we label these eigenvalues as follows:

$$\mu_n(AP) \leqslant \mu_{n-1}(AP) \leqslant \cdots \leqslant \mu_1(AP) < 0 < \gamma_1(AP) \leqslant \gamma_2(AP) \leqslant \cdots$$
$$\cdots \leqslant \gamma_{N-n}(AP) \tag{14}$$

Implicit in (14) is the assertion that AP has exactly n negative and $N-n$ positive eigenvalues. This follows from Sylvester's law of inertia or the min-max principle and we omit the proof. Note that the labeling in (14), in contrast to that in (4), is "from zero outward."

For $1 \leqslant k \leqslant n$ we define

$$\tilde{\sigma}_{(k)}(AP) \equiv \sum_{j=1}^{k} \mu_j(AP) \tag{15}$$

For $1 \leqslant k \leqslant N-n$

$$\tilde{\sigma}^{(k)}(AP) \equiv \sum_{j=1}^{k} \gamma_j(AP) \tag{16}$$

Our main theorem, which contrasts the AP problem with (9)–(13), is the following.

Theorem. Let $A \in \mathscr{H}_N$ be nonsingular with $n \leqslant N$ negative eigenvalues. Let $P \in \mathscr{P}_N$. Then

$$P \mapsto \tilde{\sigma}_{(k)}(AP) \text{ is convex and decreasing} \tag{17}$$

$$P \mapsto \tilde{\sigma}^{(k)}(AP) \text{ is concave and increasing} \tag{18}$$

$$P \mapsto \sigma_0(P^{1/2}AP^{1/2}) = \tilde{\sigma}_{(n)}(AP) = \sigma(AP) \text{ is convex and decreasing} \tag{19}$$

$$P \mapsto \sigma^0(P^{1/2}AP^{1/2}) = \tilde{\sigma}^{(N-n)}(AP) \text{ is concave and increasing} \tag{20}$$

$$P \mapsto \mu_j(AP) \text{ is decreasing and } P \mapsto \gamma_j(AP) \text{ is increasing} \tag{21}$$

Remark. In contrast to the fact that the largest negative eigenvalue of AP is convex in P, the smallest negative eigenvalue is *not* concave in P. The $n=1$ case shows this clearly. Also, there does not appear to be an analogue of (11) and (12) with $c \neq 0$ in the AP case.

The theorem is an immediate consequence of the following variational characterization of the eigenvalues of AP. The derivation of (17), for example, from (22) and (24) is easy: (22) implies that each $\mu_j(AP)$ in $\sigma_{(k)}(AP)$ is decreasing, while (24) displays $\tilde{\sigma}_{(k)}(AP)$ as the supremum of a family of linear functions.

Lemma. The negative eigenvalues $\mu_j(AP)$ are characterized by the following min-max principle:

$$\mu_j(AP) = \min_{\mathscr{K}_{j-1}} \max_{\psi} \left\{ \frac{(\psi, P\psi)}{(\psi, A^{-1}\psi)} : \psi \in \mathbf{C}^N, (\psi, A^{-1}\psi) < 0, \psi \perp \mathscr{K}_{j-1} \right\} \tag{22}$$

Here $(\cdot, \cdot)$ is the usual inner product in $\mathbf{C}^N$, $\mathscr{K}_{j-1}$ is any $(j-1)$-dimensional subspace of $\mathbf{C}^N$, and the orthogonality $\perp$ is the usual one, i.e., $(\psi, \phi) = 0$ for all $\phi \in \mathscr{K}_{j-1}$. The positive eigenvalues are characterized by

$$\gamma_j(AP) = \max_{\mathscr{K}_{j-1}} \min_{\psi} \left\{ \frac{(\psi, P\psi)}{(\psi, A^{-1}\psi)} : \psi \in \mathbf{C}^N, (\psi, A^{-1}\psi) > 0, \psi \perp \mathscr{K}_{j-1} \right\} \tag{23}$$

The eigenvalue sums $\tilde{\sigma}_{(k)}$ and $\sigma^{(k)}$ are given by

$$\tilde{\sigma}_{(k)}(AP) = \max \left\{ -\sum_{i=1}^{k} (\psi_i, P\psi_i) : \psi_i \in \mathbf{C}^N, (\psi_i, A^{-1}\psi_j)|_{i,j=1}^{k} \leqslant -\mathbf{I}_k \right\} \tag{24}$$

$$\tilde{\sigma}^{(k)}(AP) = \min \left\{ \sum_{i=1}^{k} (\psi_i, P\psi_i) : \psi_i \in \mathbf{C}^N, (\psi_i, A^{-1}\psi_j)|_{i,j=1}^{k} \geqslant \mathbf{I}_k \right\} \tag{25}$$

The requirement $(\psi_i, A^{-1}\psi_j)|_{i,j=1}^{k} \geqslant \mathbf{I}_k$ is meant in the form sense, i.e., the $k \times k$ Hermitian matrix with elements $(\psi_i, A^{-1}\psi_j) - \delta_{ij}$ is nonnegative definite.

Proof. If suffices to prove (22) and (24), because (23) and (25) follow from this by replacing A by $-A$.

To prove (22), let $H = P^{1/2}AP^{1/2}$ and $M = P^{-1/2}A^{-1}P^{-1/2} = H^{-1}$. Since $\mu_j(AP)$ is the jth negative eigenvalue of H counting downward from zero, it follows that $\{\mu_j(AP)\}^{-1} = \lambda_j(M)$ in the usual ordering, (4), of the eigenvalues of M. By the usual max-min principle,

$$\lambda_j(B) = \max_{\mathscr{K}_{j-1}} \min_{\phi} \left\{ \frac{(\phi, M\phi)}{(\phi, \phi)} : 0 \neq \phi \in \mathbf{C}^N, \phi \perp \mathscr{K}_{j-1} \right\} \tag{26}$$

$$= \max_{\mathscr{K}_{j-1}} \min_{\psi} \left\{ \frac{(\psi, A^{-1}\psi)}{(\psi, P\psi)} : (\psi, A^{-1}\psi) < 0, \psi \perp \mathscr{K}_{j-1} \right\} \tag{27}$$

Equation (27) follows from (26) by setting $\psi = P^{1/2}\phi$ and by noting that the set of ϕ's in (26) can be restricted to those satisfying the additional condition $(\phi, M\phi) < 0$; this is possible because $\lambda_j(M) < 0$ and hence, for every $\mathscr{K}_{j-1}$, there is a ϕ for which $(\phi, M\phi) < 0$. Now, for any family F of negative reals we have

$$\frac{1}{\sup\{x \in F\}} = \inf \left\{ \frac{1}{x} : \quad x \in F \right\} \tag{28}$$

By applying (28) twice to (27), we obtain (17).

To prove (24), we first remark that the right side of (24) (call it $X_{(k)}$) is

$$X_{(k)} = -\min \left\{ \sum_{i=1}^{k} (\phi_i, H^2\phi_i) : (\phi_i, H\phi_j)|_{i,j=1}^{k} \leqslant -\mathbf{I}_k \right\} \tag{29}$$

This follows from (24) by setting $\psi_j = AP^{1/2}\phi_j$. Let Π denote the orthogonal projector onto $\mathbf{B}^n \subset \mathbf{C}^N$, the negative eigenspace of H. We can then write $\phi_j = f_j + g_j$ with $f_j = \Pi\psi_j$, $g_j = \psi_j - \Pi\psi_j$. Consequently, $(\phi_i, H\phi_j) = (f_i, Hf_j) + (g_i, Hg_j)$ and, in the sense of forms,

$$(f_i, Hf_j)|_{i,j=1}^{k} \leqslant -\mathbf{I}_k \tag{30}$$

since $(\phi_i, H\phi_j)|_{i,j=1}^{k} \leqslant -\mathbf{I}_k$ and (g_i, Hg_j) is nonnegative definite. Likewise

$$(\phi_i, H^2\phi_i) = (f_i, H^2 f_i) + (g_i, H^2 g_i) \geqslant (f_i, H^2 f_i) \tag{31}$$

From (30) and (31) we see that matters are improved by replacinig ϕ_i by $\Pi\phi_i$, and hence

$$X_{(k)} = -\min\left\{\sum_{i=1}^{k} (\phi_i, L^2\phi_i) \;:\; (\phi_i, L\phi_j)|_{i,j=1}^{k} \geqslant \mathbf{I}_k,\ \phi_i \in \mathbf{B}^n \subset \mathbf{C}^N\right\} \tag{32}$$

with $L \equiv -\Pi H \Pi \geqslant 0$. The usual variational principle can be stated in the following generalized form for matrices $\hat{L} \in \mathscr{P}_n$:

$$\sigma_{(k)}(\hat{L}) = \min\left\{\sum_{i=1}^{k} (\chi_i, \hat{L}^2\chi_i) \;:\; (\chi_i, \hat{L}\chi_j)|_{i,j=1}^{k} \geqslant \mathbf{I}_k,\ \chi_i \in \mathbf{C}^n\right\} \tag{33}$$

By a change of basis, the min $\{\cdot\}$ in (32) is the same as the min $\{\cdot\}$ in (33) with $\hat{L}$ taken to be the restriction of L to its invariant subspace $\mathbf{B}^n$. Thus, $X_{(k)} = -\sigma_{(k)}(\hat{L}) = \tilde{\sigma}_{(k)}(AP)$. ▌

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