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The functional calculus and a generalization of the Coulson–Rushbrooke pairing theorem*

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Fundamental techniques of functional calculus have been applied to elucidate the symmetric properties of the spectra of certain operators on Hilbert spaces. The main theorem provides, in a broader context, yet another proof of the Coulson–Rushbrooke pairing theorem. The necessary features of the functional calculus are explained in some detail.

1. Introduction

Our purpose in this note is to display how one can use in mathematical chemistry what is known as the functional calculus for operators on Hilbert spaces. Functional calculus is a powerful mathematical tool which can deal with both matrices and operators on abstract spaces; it leads one to a broader perspective which conventional methods fail to provide. We will illustrate this by applying the functional calculus for a generalization of the Coulson–Rushbrooke pairing theorem to compact operators. By restricting our argument to matrices, we obtain yet another proof of the usual pairing theorem. The power of the functional calculus and related techniques of functional analysis has also been demonstrated by recent studies of the asymptotic linearity theorem [1–3].

Section 2 is devoted to operators on Hilbert space, the functional calculus and the spectral theorem for compact normal operators.

In section 3, we study the space of continuous functions on a compact subset of $\mathbb{C}$ and derive as a consequence of the celebrated Stone–Weierstrass theorem that the odd polynomials are dense in the space of odd continuous functions.

In section 4, we formulate and prove the pairing theorem for compact normal operators using the functional calculus and the technical result of section 3. The

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final section is devoted to some concluding remarks. A short appendix is included on trace class operators to explain several elementary properties which are used in the proof of the main theorem in section 4.

2. Functional calculus and the spectral theorem

Let $\mathcal{H}$ be a complex Hilbert space with an inner product $\langle\ ,\ \rangle$ which is linear in the first variable and conjugate linear in the second variable. Let $\mathcal{B}(\mathcal{H})$ denote the space of bounded linear operators on $\mathcal{H}$. For $T \in \mathcal{B}(\mathcal{H})$, there exists a unique $T^* \in \mathcal{B}(\mathcal{H})$ such that $\langle T\xi, \eta\rangle = \langle \xi, T^*\eta\rangle$, for all ξ, $\eta \in \mathcal{H}$. T^* is called the adjoint of T and T is called self-adjoint if $T^* = T$. An operator T which commutes with its adjoint (that is, $T^*T = TT^*$) is called normal.

For any $T \in \mathcal{B}(\mathcal{H})$, let $\sigma(T) = \{\lambda \in \mathbb{C} : \lambda I - T \text{ is not invertible}\}$, where I is the identity operator, $I\xi = \xi$, for all $\xi \in \mathcal{H}$. Then $\sigma(T)$ is called the spectrum of T and it is always a non-empty compact subset of $\mathbb{C}$. If $\mathcal{H}$ is finite dimensional, then $\sigma(T)$ consists of all the eigenvalues of T. For infinite dimensional $\mathcal{H}$, however, elements of $\sigma(T)$ need not be eigenvalues. There is an important class of operators, called compact operators, for which every non-zero element of $\sigma(T)$ is an eigenvalue and for such operators, the spectral theory is very similar to the finite dimensional case.

An operator T in $\mathcal{B}(\mathcal{H})$ is called compact if $\{T\xi : \xi \in \mathcal{H}, \|\xi\| \leq 1\}$ has compact closure in $\mathcal{H}$. Here, $\|\xi\| = \langle \xi, \xi\rangle^{1/2}$, for $\xi \in \mathcal{H}$. For basic information on compact operators, see Dunford and Schwartz [4].

2.1. SPECTRAL THEOREM FOR COMPACT NORMAL OPERATORS

Let $T \in \mathcal{B}(\mathcal{H})$ be compact and normal. For $\lambda \in \mathbb{C}$, let

$$V_\lambda = \{\xi \in \mathcal{H} : T\xi = \lambda\xi\}. \tag{1}$$

Each V_λ is a closed subspace of $\mathcal{H}$. If $\lambda \neq 0$, then V_λ is finite dimensional and $\lambda \in \sigma(T)$ if and only if $V_\lambda \neq \{0\}$. $\sigma(T)$ is a countable set and, if it is infinite, the non-zero elements of $\sigma(T)$ can be enumerated as $\{\lambda_j : j = 1, 2, \ldots\}$ so that $|\lambda_1| \geq |\lambda_2| \geq \ldots$ and $\lim_{j\to\infty} \lambda_j = 0$. If $\sigma(T)$ is a finite set, then let $\sigma(T)\setminus\{0\} = \{\lambda_1, \ldots, \lambda_n\}$ be an enumeration. For each j, let E_j denote the orthogonal projection of $\mathcal{H}$ onto V_{λ_j}. Then $E_iE_j = 0$, if $i \neq j$ and

$$T = \sum_j \lambda_j E_j. \tag{2}$$

The representation of T in (2) is unique up to some permutations of the order of terms.

Before we formally describe the functional calculus of normal operators, let us point out some consequences of the representation in (2). With T given as in (2) and k a positive integer:

$$T^k = \sum_j \lambda_j^k E_j \quad \text{and} \quad (T^*)^k = \sum_j \bar{\lambda}_j^k E_j. \tag{3}$$

Thus, if $p(z) = \sum_{k,l=0}^m a_{k,l} z^k \bar{z}^l$ is a polynomial in z and $\bar{z}$ with $a_{k,l} \in \mathbb{C}$ for $0 \le k, l \le m$ and $p(T)$ is interpreted as

$$p(T) = \sum_{k,l=0}^{m} a_{k,l}\, T^k (T^*)^l, \tag{4}$$

then, using (2), $p(T) = \sum_j p(\lambda_j) E_j$. This illustrates how, for fixed T, one may associate different operators $\phi(T)$ to different functions ϕ on the spectrum of T. This is called the functional calculus and the class of functions used can be much larger than the polynomials. Moreover, it is not necessary to assume that the operator T is compact.

2.2. FUNCTIONAL CALCULUS FOR NORMAL OPERATORS

Let $T \in \mathcal{B}(\mathcal{H})$ be a normal operator. The operator norm of T is given by

$$\|T\| = \sup\{\|T\xi\| : \xi \in \mathcal{H},\ \|\xi\| \le 1\}. \tag{5}$$

Then $|\lambda| \le \|T\|$ for all $\lambda \in \sigma(T)$. In fact,

$$\sup\{|\lambda| : \lambda \in \sigma(T)\} = \|T\|, \tag{6}$$

since T is normal ([5], 4.1.1). Let $C(\sigma(T))$ denote the space of all continuous complex-valued functions on $\sigma(T)$. Any complex polynomial $p(z) = \sum_{k,l=0}^m a_{k,l}\, z^k \bar{z}^l$ in z and $\bar{z}$ can be considered as an element of $C(\sigma(T))$. Let $\mathcal{P}$ denote the set of all such polynomials. For $f \in C(\sigma(T))$, let $\|f\|_\infty = \sup\{|f(z)| : z \in \sigma(T)\}$. Then $C(\sigma(T))$ equipped with $\|\cdot\|_\infty$ is a Banach space and the Stone–Weierstrass theorem ([6], 7.34) implies that $\mathcal{P}$ is dense in $C(\sigma(T))$ with this norm.

For each $p \in \mathcal{P}$, $p(T) \in \mathcal{B}(\mathcal{H})$ is naturally defined as in (4) and the map $p \to p(T)$ is a linear map of $\mathcal{P}$ into $\mathcal{B}(\mathcal{H})$ such that $\|p(T)\| = \|p\|_\infty$, for all $p \in \mathcal{P}$.

Now, for any $\phi \in C(\sigma(T))$ let $(p_n)_{n=1}^\infty$ be a sequence in $\mathcal{P}$ such that $\|p_n - \phi\|_\infty \to 0$. This implies, in particular, that $(p_n)_{n=1}^\infty$ is a Cauchy sequence; that is, $\|p_n - p_m\|_\infty \to 0$, as $n, m \to \infty$. Thus,

$$\|p_n(T) - p_m(T)\| = \|(p_n - p_m)(T)\| = \|p_n - p_m\|_\infty \to 0, \quad \text{as } n, m \to \infty, \tag{7}$$

in $\mathcal{B}(\mathcal{H})$. Since $\mathcal{B}(\mathcal{H})$ is complete, there exists an operator, called $\phi(T)$, in $\mathcal{B}(\mathcal{H})$ such that $p_n(T) \to \phi(T)$. It is easily verified that $\phi(T)$ is well defined in the sense that if $(p_n')_{n=1}^\infty$ is any other sequence in $\mathcal{P}$ converging to ϕ, then $p_n'(T) \to \phi(T)$ as well. The fact that $\phi(T)$ can be given meaning for any continuous function ϕ on $\sigma(T)$ is called the functional calculus of T. For complete proofs of the properties listed below, the reader is referred to chapter 5 of Kadison and Ringrose [5].

2.3. PROPERTIES OF THE FUNCTIONAL CALCULUS

(i) $\phi(T)$ is normal for all $\phi \in C(\sigma(T))$.

(ii) The map $\phi \to \phi(T)$, from $C(\sigma(T))$ into $\mathcal{B}(\mathcal{H})$, is a linear isometry. (Isometry here means that $\|\phi(T)\| = \|\phi\|_\infty$, for all $\phi \in C(\sigma(T))$.)

(iii) If $S \in \mathcal{B}(\mathcal{H})$ and $ST = TS$, then $S\phi(T) = \phi(T)S$, for all $\phi \in C(\sigma(T))$. That is, $\phi(T)$ commutes with every operator which commutes with T.

(iv) For $\phi \in C(\sigma(T))$, $\phi(T)^* = \overline{\phi}(T)$.

(v) For ϕ, $\psi \in C(\sigma(T))$, $(\phi\psi)(T) = \phi(T)\psi(T)$.

(vi) If ϕ is the restriction to $\sigma(T)$ of a function which is holomorphic on some disk in $\mathbb{C}$, centered at 0 and containing $\sigma(T)$, then ϕ is given by a power series $\phi(z) = \sum_{n=1}^{\infty} a_n z^n$. In that case, $\phi(T) = \sum_{n=0}^{\infty} a_n T^n$, in the sense that

$$\|\phi(T) - \sum_{n=0}^{m} a_n T^n\| \to 0, \quad \text{as } m \to \infty,$$

where $T^0 = I$. Thus, we have for example

$$\exp(T) = \sum_{n=0}^{\infty} \frac{1}{n!} T^n.$$

(vii) If T is a compact normal operator with spectral decomposition $T = \sum_j \lambda_j E_j$ and $\phi \in C(\sigma(T))$, then

$$\phi(T) = \sum_j \phi(\lambda_j) E_j.$$

The next three remarks are made to illustrate a more abstract way of viewing the functional calculus and are given without a detailed explanation of the terminology. For complete details, we again refer the reader to ref. [5], chapter 5.

2.4. REMARKS

(1) Properties (ii), (iv) and (v) in 2.3 collectively state that $\phi \to \phi(T)$ is an isometric $*$-isomorphism of the C^*-algebra $C(\sigma(T))$ onto the smallest C^*-algebra in $\mathcal{B}(\mathcal{H})$ which contains T and I, denoted $C^*(T)$. Thus, as C^*-algebras, $C(\sigma(T))$ and $C^*(T)$ are exactly the same and $C^*(T) = \{\phi(T) : \phi \in C(\sigma(T))\}$.

(2) For a normal operator T, there is a spectral decomposition which generalizes 1. If T is normal, then there exists a unique projection-valued measure E on the Borel subsets of $\sigma(T)$ (thus, $E(B)$ is a projection in $\mathcal{B}(\mathcal{H})$ for each Borel subset $B \subseteq \sigma(T)$) such that $T = \int_{\sigma(T)} \lambda \, \mathrm{d}E(\lambda)$. The interpretation of this formula is

as follows: for $\xi \in \mathcal{H}$, an ordinary Borel measure E_ξ is defined by $E_\xi(B) = \langle E(B)\xi, \xi\rangle$, for all Borel subsets B of $\sigma(T)$ and $\langle T\xi, \xi\rangle = \int_{\sigma(T)} \lambda \, \mathrm{d}E_\xi(\lambda)$.

With this spectral decomposition, then, for $\phi \in C(\sigma(T))$,

$$\phi(T) = \int_{\sigma(T)} \phi(\lambda) \; \mathrm{d}E(\lambda). \tag{8}$$

(3) The functional calculus can be extended to a larger class of functions on $\sigma(T)$. A complex-valued function ϕ on $\sigma(T)$ is called Borel measurable if $\phi^{-1}(U)$ is a Borel set for each open subset U of $\mathbb{C}$. If ϕ is a bounded Borel measurable function on $\sigma(T)$, then $\int_{\sigma(T)} \phi(\lambda) \, \mathrm{d}E(\lambda)$ defines a bounded operator on $\mathcal{H}$ which can be denoted $\phi(T)$. Properties (i) to (v) above hold for bounded Borel measurable functions, except that in (ii) the norm on the space of bounded Borel functions must be modified to be the essential supremum norm with respect to the null sets defined by the projection-valued measure E.

3. Odd polynomials and continuous functions

For $r > 0$, let $D_r = \{z \in \mathbb{C} : |z| \le r\}$. We will usually be concerned with D_r, for some $r \ge \|T\|$ and some operator T, so that $\sigma(T) \subseteq D_r$. Then any $\phi \in C(D_r)$ defines a unique element of $C(\sigma(T))$ by restriction to $\sigma(T)$, so $\phi(T)$ makes sense. Of course, if $\|\phi\|_{D_r} = \sup\{z \in D_r : |\phi(z)|\}$, then we are only assured of the inequality $\|\phi(T)\| \le \|\phi\|_{D_r}$. We are moving to the disk D_r simply so that the domain is invariant under multiplication by -1.

Again, let $\mathcal{P}$ denote the space of polynomials in z and $\bar{z}$ and consider $\mathcal{P}$ as a subspace of $C(D_r)$.

A function $\phi \in C(D_r)$ is called odd if $\phi(-z) = -\phi(z)$, for all $z \in D_r$. Let $C_{\text{odd}} = \{\phi \in C(D_r) : \phi \text{ is odd}\}$ and let $\mathcal{P}_{\text{odd}} = \mathcal{P} \cap C_{\text{odd}}$. Both C_{odd} and $\mathcal{P}_{\text{odd}}$ are subspaces of $C(D_r)$ and C_{odd} is easily seen to be closed. It is also easy to check that any $p \in \mathcal{P}_{\text{odd}}$ is of the form

$$p(z) = \sum_{\substack{j,k=0 \\ j+k \text{ odd}}} a_{j,k} z^j \bar{z}^k, \quad \text{for} \quad a_{j,k} \in \mathbb{C}, \; 1 \le j, \; k \le n, \tag{9}$$

with $j + k$ odd.

We are now ready to state and prove the main proposition of this section.

PROPOSITION 3.1

$\mathcal{P}_{\text{odd}}$ is dense in C_{odd}.

Proof

Define a linear map O on $C(D_r)$ by

$$[O(\phi)](z) = \frac{1}{2}(\phi(z) - \phi(-z)). \tag{10}$$

Then O is a linear map of $C(D_r)$ onto C_{odd} satisfying

(a) $O(\phi) = \phi$ if and only if $\phi \in C_{\text{odd}}$.

(b) $O(\mathcal{P}) = \mathcal{P}_{\text{odd}}$.

(c) $\| O(\phi) \|_{D_r} \leq \| \phi \|_{D_r}$, for all $\phi \in C(D_r)$.

Now, suppose $\phi \in C_{\text{odd}}$ and $\varepsilon > 0$. By the Stone–Weierstrass theorem, there exists $p \in \mathcal{P}$ such that $\|\phi - p\|_{D_r} < \varepsilon$. Let $p_0 = O(p) \in \mathcal{P}_{\text{odd}}$. Then, using (a), (b) and (c),

$$\|\phi - p_0\|_{D_r} = \|O(\phi) - O(p)\|_{D_r} = \|O(\phi - p)\|_{D_r} \leq \|\phi - p\|_{D_r} < \varepsilon. \tag{11}$$

Since $\varepsilon > 0$ was arbitrary, $\mathcal{P}_{\text{odd}}$ is dense in C_{odd}.

4. A pairing theorem for compact normal operators

In this section, we will use the approximation result for odd continuous functions from the previous section and the functional calculus to prove a pairing theorem for compact normal operators. Pairing properties for the eigenvalues and eigenvectors of operators which satisfy certain commutation relations that generalize those satisfied by the adjacency matrices of alternant hydrocarbons have been discussed in ref. [7]. A quite general theory of such operators has been developed by Zivković in ref. [8] and references therein. Our main purpose here is to illustrate the role which can be played by the functional calculus.

Before formulating the statement of our theorem, let us consider the usual finite dimensional theorem to find the appropriate hypothesis.

The usual pairing theorem concerns the adjacency matrix of a bipartite graph. If the vertices of the graph are partitioned into two subsets of k and $n - k$ elements, respectively, so that no two vertices in the same subset are joined in the graph, then, by listing the k-elements of the first subset followed by the $n - k$ elements of the second subset, the adjacency matrix A is of the form:

$$A = \begin{pmatrix} O_k & B \\ C & O_{n-k} \end{pmatrix}, \tag{12}$$

where O_j denotes the $j \times j$ zero matrix, B is a $k \times (n-k)$ matrix and C is a $(n-k) \times k$ matrix. In fact, here A is symmetric, so $C = B^t$. Then A is self-adjoint and the pairing theorem states that, for $\lambda \in \mathbb{R}$, λ is an eigenvalue of A if and only if $-\lambda$ is an eigenvalue of A and the dimensions of the eigenspaces for λ and $-\lambda$ are equal.

This theorem has been extensively investigated for matrices (see the survey article [9] and theorem 3.11 of ref. [10]) and it is now known that an adjacency matrix A in $M_n(\mathbb{C})$ can be put in the form (12) if and only if the characteristic polynomial p_A of A is of the form $p_A(\lambda) = \lambda^l q(\lambda^2)$, for some polynomial q and $l \geq 0$ [10]. This form of the characteristic polynomial easily implies the pairing theorem.

Since we are interested in generalizing to operators, it is necessary to express the condition of (12) in a basis-free manner. If we let

$$P = \begin{pmatrix} I_k & O_{k,n-k} \\ O_{n-k,k} & O_{n-k} \end{pmatrix}, \tag{13}$$

where I_k is the $k \times k$ identity matrix, then P, acting as a linear transformation of $\mathbb{C}^n$ is an orthogonal projection of $\mathbb{C}^n$ onto a k-dimensional subspace and

$$PAP = (I_n - P)A(I_n - P) = O_n. \tag{14}$$

The existence of such a P is the property which we generalize to arbitrary Hilbert space.

A projection in $\mathcal{B}(\mathcal{H})$ is an operator $P \in \mathcal{B}(\mathcal{H})$ such that $P^2 = P$ and $P^* = P$. Recall that I denotes the identity operator on $\mathcal{H}$ and we will simply use O to denote the zero operators on $\mathcal{H}$. We are now ready to state and prove a pairing theorem for compact normal operators.

THEOREM

Let T be a compact normal operator on a Hilbert space $\mathcal{H}$. For each $\lambda \in \mathbb{C}$, let $V_\lambda = \{\xi \in \mathcal{H}: T\xi = \lambda\xi\}$. Suppose that there exists a projection P in $\mathcal{B}(\mathcal{H})$ such that $PTP = O$ and $(I-P)T(I-P) = O$. Then the dimension of $V_{-\lambda}$ is equal to the dimension of V_λ for all $\lambda \in \mathbb{C}$.

Proof

Consider the following closed subspaces of $\mathcal{B}(\mathcal{H})$:

$$\mathcal{W} = \{PS(I-P) + (I-P)RP : S,\ R \in \mathcal{B}(\mathcal{H})\} \tag{15}$$

and

$$\mathcal{A} = \{PSP + (I-P)R(I-P) : S,\ R \in \mathcal{B}(\mathcal{H})\}. \tag{16}$$

The $\mathcal{A}$ and $\mathcal{W}$ are complementary subspaces of $\mathcal{B}(\mathcal{H})$ (that is, $\mathcal{A} + \mathcal{W} = \mathcal{B}(\mathcal{H})$ and $\mathcal{A} \cap \mathcal{W} = \{0\}$) which satisfy:

(i) $\mathcal{A}\mathcal{A} = \mathcal{A}$ ($\mathcal{A}$ is a subalgebra).

(ii) $\mathcal{A}\mathcal{W} \subseteq \mathcal{W}$ and $\mathcal{W}\mathcal{A} \subseteq \mathcal{W}$,

(iii) $\mathcal{W}\mathcal{W} \subseteq \mathcal{A}$,

(iv) $\mathcal{W}^* = \mathcal{W}$ and $\mathcal{A}^* = \mathcal{A}$,

(v) $\mathcal{W}^{2l+1} \subseteq \mathcal{W}$, for all $l = 0, 1, 2, \ldots$.

Each of these properties (i)–(v) are easily verified.

Note that $T \in \mathcal{W}$, since

$$\begin{aligned} T &= ((I-P)+P)\,T((I-P)+P) \\ &= PT(I-P) + (I-P)TP. \end{aligned} \tag{17}$$

Using (iv) and (v) and the fact that $\mathcal{W}$ is a subspace of $\mathcal{B}(\mathcal{H})$, one sees that $p(T) \in \mathcal{W}$, for any odd polynomial p. Let $r = \|T\|$ and let ϕ be an odd continuous function on D_r. That is $\phi \in C_{\text{odd}}$, in the notation of section 3. Using 3.1, choose a sequence $\{p_n\}_{n=1}^{\infty}$ of odd polynomials so that $\|p_n - \phi\|_{D_r} \to 0$. Since $\sigma(T) \subseteq D_r$, one has $\sup_{z \in \sigma(T)} |\psi(z)| \leq \|\psi\|_{D_r}$, for any $\psi \in C(D_r)$. Thus, 2.3(ii) implies that $\|p_n(T) - \phi(T)\| \to 0$. Since each $p_n(T) \in \mathcal{W}$ and $\mathcal{W}$ is closed in the norm topology, $\phi(T) \in \mathcal{W}$, for any odd continuous function ϕ defined on a disk D_r which contains $\sigma(T)$.

Recall from 2.3(vii) that, if T has spectral representation,

$$T = \sum_i \lambda_i E_{\lambda_i}, \tag{18}$$

then

$$\phi(T) = \sum_i \phi(\lambda_i) E_{\lambda_i} \tag{19}$$

for any $\phi \in C(D_r)$. If there exists an $\varepsilon > 0$ such that $\phi(z) = 0$ for $|z| < \varepsilon$, then $\phi(\lambda_i) \neq 0$, for only finitely many λ_i due to the fact that if there are infinitely many λ_i, then $\lambda_i \to 0$ (see 2.3). Also, by 2.3, each E_{λ_i}, for $\lambda_i \neq 0$, is of finite rank. Thus, $\phi(T)$ is of finite rank if ϕ vanishes on a neighbourhood of 0 in $\mathbb{C}$. Finite rank operators are of trace class. Trace class operators are discussed in the appendix and we will use the properties described there without reference. If $S \in \mathcal{W}$ and S is also a trace class operator, then trace$(S) = 0$, since

$$\begin{aligned} \text{trace}(S) &= \text{trace}(PS(I-P) + (I-P)SP) \\ &= \text{trace}(PS(I-P)) + \text{trace}((I-P)SP) \\ &= \text{trace}((I-P)PS) + \text{trace}(P(I-P)S) \\ &= \text{trace}(0) + \text{trace}(0) = 0. \end{aligned} \tag{20}$$

To sum up the previous discussion, if ϕ is an odd continuous function on D_r which vanishes on a neighbourhood of 0, then $\phi(T)$ is in $\mathcal{W}$, of trace class and trace$(\phi(T)) = 0$. On the other hand,

$$\operatorname{trace}(\phi(T)) = \sum_i \phi(\lambda_i)\ \operatorname{rank}(E_{\lambda_i})$$

$$= \sum_{i,\phi(\lambda_i)\neq 0} \phi(\lambda_i)\ \dim(V_{\lambda_i}), \tag{21}$$

where $\dim(V_{\lambda_i})$ denotes the dimension of V_{λ_i}.

Now for any $\lambda \in \sigma(T)$, $\lambda \neq 0$, by 2.1, there exists an $\varepsilon > 0$ such that $|\lambda| > 2\varepsilon$ and if $\mu \in \sigma(T)$, $\mu \neq \pm\lambda$, then $|\mu - \lambda| > \varepsilon$ and $|\mu + \lambda| > \varepsilon$. That is, the ε-disks around λ and $-\lambda$ contain no other points in $\sigma(T)$. Note that we have not yet shown that $-\lambda \in \sigma(T)$. Let $\phi \in C_{\mathrm{odd}}$ such that $\phi(\lambda) = 1$ (so $\phi(-\lambda) = -1$) and such that $\phi(z) = 0$ if $|z - \lambda| \geq \varepsilon$ and $|z + \lambda| \geq \varepsilon$. Then, by the above discussion,

$$0 = \operatorname{trace}(\phi(T)) = \sum_{i,\phi(\lambda_i)\neq 0} \phi(\lambda_i)\ \dim(V_{\lambda_i}),$$

$$= \dim(V_\lambda) - \dim(V_{-\lambda}). \tag{22}$$

Thus, $\dim(V_\lambda) = \dim(V_{-\lambda})$, for any $\lambda \in \sigma(T)$, $\lambda \neq 0$. It is clear that $\dim(V_\lambda) = \dim(V_{-\lambda})$, for all other points λ in $\mathbb{C}$. □

5. Summary

Our purpose in this paper is to introduce the power of the functional calculus to mathematically inclined chemists. We have demonstrated this by proving a version of the Coulson–Rushbrooke pairing theorem for compact normal operators on a Hilbert space. When the Hilbert space is finite dimensional, we obtain a new proof of the matrix version of the pairing theorem. There are certainly more elementary, combinatorially based, proofs for the matrix version and there may even be simpler proofs for our infinite dimensional, compact operator version. However, we believe that there is great potential for dealing with certain mathematical problems of special interest to chemists by using the functional calculus. Even for questions on the spectra of matrices, this way of thinking can be valuable.

To briefly sum up the functional calculus: if A is a bounded normal operator on a Hilbert space (or a normal matrix) and $\sigma(A)$ denotes the spectrum of A, then, for any continuous complex-valued function ϕ on $\sigma(A)$, $\phi(A)$ has a precise meaning and the map $\phi \rightarrow \phi(A)$ gives you an exact copy of $C(\sigma(A))$ inside the space of bounded normal operators (or matrices). This allows the use of special knowledge about continuous functions to obtain information about A, $\sigma(A)$ and $\phi(A)$, for particular functions ϕ of interest.

Appendix. Trace class operators

The trace is a valuable tool in the study of finite dimensional matrices and can be useful in operator theory as long as the operators of interest lie in a special class called the trace class. A very readable, but rigorous treatment of the trace class operators is given in ref. [11], where the reader is directed for complete details of what follows.

Let $\mathcal{H}$ be a Hilbert space and let $\{\xi_\alpha\}_{\alpha\in\Delta}$ be a fixed orthonormal basis for $\mathcal{H}$. Let $A \in \mathcal{B}(\mathcal{H})$. If $\sum_{\alpha\in\Delta}\|A\xi_\alpha\|^2 < \infty$, then A is called a Hilbert–Schmidt operator. If $\{\eta_\beta\}_{\beta\in\Gamma}$ is any other orthonormal basis of $\mathcal{H}$, then $\sum_{\beta\in\Gamma}\|A\eta_\beta\|^2 = \sum_{\alpha\in\Delta}\|A\xi_\alpha\|^2$, so the definition is independent of the basis. If A and B are both Hilbert–Schmidt operators, then $\sum_{\alpha\in\Delta}\langle A\xi_\alpha, B\xi_\alpha\rangle$ converges absolutely and, again, the sum is independent of the particular orthonormal basis which has been chosen. Hilbert–Schmidt operators are interesting and important in their own right; however, here we use them to define the trace class.

If $A = C^*B$, with B and C Hilbert–Schmidt operators, then, for any orthonormal basis $\{\xi_\alpha\}_{\alpha\in\Delta}$,

$$\sum_{\alpha\in\Delta}\langle A\xi_\alpha, \xi_\alpha\rangle = \sum_{\alpha\in\Delta}\langle B\xi_\alpha, C\xi_\alpha\rangle \tag{23}$$

converges absolutely and is independent of the basis. An operator $A \in \mathcal{B}(\mathcal{H})$ is called a trace class operator if A can be written as $A = C^*B$, with B and C Hilbert–Schmidt operators. Let $\mathcal{TC}(\mathcal{H})$ denote the set of all trace class operators on $\mathcal{H}$.

If $A \in \mathcal{TC}(\mathcal{H})$, let

$$\mathrm{trace}(A) = \sum_{\alpha\in\Delta}\langle A\xi_\alpha, \xi_\alpha\rangle, \tag{24}$$

where $\{\xi_\alpha\}_{\alpha\in\Delta}$ is any orthonormal basis for $\mathcal{H}$. The following properties of $\mathcal{TC}(\mathcal{H})$ can all be found in chapter III of ref. [11].

PROPERTIES OF TRACE CLASS OPERATORS

(i) $\mathcal{TC}(\mathcal{H})$ is a linear subspace of $\mathcal{B}(\mathcal{H})$.

(ii) $A \in \mathcal{TC}(\mathcal{H})$ implies $A^* \in \mathcal{TC}(\mathcal{H})$.

(iii) $A \in \mathcal{TC}(\mathcal{H})$ and $B \in \mathcal{B}(\mathcal{H})$ implies AB, $BA \in \mathcal{TC}(\mathcal{H})$.

(iv) $\mathrm{trace} : \mathcal{TC}(\mathcal{H}) \to \mathbb{C}$ is a linear functional.

(v) $A \in \mathcal{TC}(\mathcal{H})$ and $B \in \mathcal{B}(\mathcal{H})$ implies

$$\mathrm{trace}(AB) = \mathrm{trace}(BA).$$

(vi) $A \in \mathcal{TC}(\mathcal{H})$, $A \neq 0$ implies

$$\mathrm{trace}(A^*A) > 0.$$

An operator $F \in \mathcal{B}(\mathcal{H})$ is called a finite rank operator if its range $F\mathcal{H}$ is finite dimensional. It is easy to verify that finite rank operators are trace class and if P is a finite rank projection, then $\mathrm{trace}(P) = \mathrm{rank}(P)$, which is the dimension of $P\mathcal{H}$.

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