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NONNEGATIVE UNITARY OPERATORS

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ABSTRACT. Unitary operators in Hilbert space map an orthonormal basis onto another. In this paper we study those that map an orthonormal basis onto itself. We show that a sequence of cardinal numbers is a complete set of unitary invariants for such an operator. We obtain a characterization of these operators in terms of their spectral properties. We show how much simpler the structure is in finite-dimensional space, and also describe the structure of certain isometries in Hilbert space.

1. Introduction

In this paper we study the structure and the unitary equivalence problem of unitary operators acting in an arbitrary (in general nonseparable) complex Hilbert space H and having the property that their infinite matrix with respect to *some* orthonormal basis in H is *entrywise* nonnegative. Fixing an arbitrary orthonormal basis E, a unitary operator U will have a nonnegative infinite matrix $M(U; E, E)$ with respect to E if and only if the matrix will contain exactly one entry 1 in each row and in each column, all other entries being 0. Since a unitary operator U can be nonnegative in this sense with respect to *no* or else w.r.t. *several* orthonormal bases, the first well-posed question should be: if U is nonnegative with respect to E, is U then unitarily equivalent to some well-defined operator from a canonical class (which should desirably be described in relatively simple terms)? We shall answer this question in Theorem 1, and see also how this operator (unitarily equivalent to U) determines a complete system of unitary invariants (the sequence c of cardinals in Theorem 1). Note that our nonnegative unitary operator U (or the corresponding nonnegative matrix) is a natural generalization of permutation matrices in finite-dimensional spaces.

The next natural question is: how can we recognize (from the spectral properties of U) whether the unitary operator U is nonnegative with respect to *some* orthonormal basis? The complete answer is given in Theorem 2 using the canonical direct sum decomposition of U into absolutely continuous, singular continuous and discrete (or point) parts and using the elements of multiplicity theory for these parts. The example of the Fourier-Plancherel operator will show that the answer

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can also be used in some cases for effectively determining bases with respect to which the given unitary operator has a nonnegative matrix.

Theorem 3 will satisfy those who had hoped that the natural characteristic (the sequence d of cardinals in Theorem 1) of the operators from the canonical class would be a complete set of unitary invariants for U. Though it is not so in general, it is in finite-dimensional spaces. We can, e.g., prove it by a really finite-dimensional argument, using the equality of the trace of matrices of an operator in different bases. Finally, in Theorem 4 we shall describe the connection between nonnegativity (of a certain type) of an isometry and of its unitary part in the von Neumann-Wold decomposition.

Questions of (entrywise) nonnegativity of matrices of normal operators in the finite-dimensional case have recently been studied in a number of papers. For an example of the treated problems and for further references see, e.g., Jain and Snyder [JS], Chen and Li [CL], Li, Hall and Zhang [LHZ] and Wang and Zhang [WZ]. A similar problem for stochastic matrices was studied by Sinkhorn [S].

We always work in Hilbert space. For characterizations of isometries in finite-dimensional l^p $(1 \leq p \leq \infty)$ spaces see, e.g., Li and So [LS], Chang and Li [CaL], Wang et al. [W] and the references therein. In possibly infinite dimensions, for the case of a surjective isometry (for $p \neq 2$) see [LT, Prop. 2.f.14, p. 112]. A complete set of invariants for positively similar positively reachable finite-dimensional linear systems has been obtained in [BCRS].

We shall list some facts from the theory of bounded linear operators in Hilbert spaces which we shall need later. Let U be a unitary operator in the Hilbert space H with resolution of the identity P, and let q denote Lebesgue measure on the unit circle C_1. Then H is the orthogonal sum of the subspaces

$$H = H_s \oplus H_a \oplus H_p$$

such that U leaves each subspace invariant, the restrictions U_s, U_a, U_p are unitary operators called the singular continuous, absolutely continuous and point (discrete) parts of U (with respect to q), and H_p is the closed subspace spanned by all the eigenvectors of the operator U. The subspaces consist of exactly those vectors $x \in H$ for which the nonnegative measure $(P(\cdot)x, x)$ is singularly continuous, absolutely continuous or discrete (with respect to q), respectively (cf. [DS3]).

Let V be an isometry in H, and let H_w be the orthogonal complement $V(H)^{\perp} \equiv H \ominus V(H)$. Then

$$H_t := H_w \oplus VH_w \oplus V^2H_w \oplus \dots$$

is a V-reducing closed subspace with complement $H_u := H \ominus H_t \equiv \bigcap_n V^n H$. The restriction $V_u := V|H_u$ is unitary, and the restriction $V_t := V|H_t$ is a multiple unilateral shift, the multiplicity of which is the orthogonal dimension of H_w (cf. [Hal2]). The orthogonal sum $V = V_u \oplus V_t$ is the *von Neumann-Wold* or canonical decomposition of V.

Let H, K be complex Hilbert spaces with orthonormal bases E, F, respectively, of arbitrary cardinalities. The operator $V : H \to K$ is said to be (E, F)-*nonnegative* if it maps each element in H with nonnegative E-coefficients into an element in K with nonnegative F-coefficients. The *infinite matrix* $M(V; E, F)$ *of* V with respect to the bases (E, F) is defined by its entries

$$v_{ij} := (Ve_j, f_i) \quad (e_j \in E, f_i \in F)$$

where (,) denotes scalar product, the corresponding index set depends on E and F (cf. [Hal2, p. 23]), and the matrix is, of course, entrywise nonnegative. If $E = F$, we shall also use the equivalent notation

$$M(V; E, E) \equiv M(V; E) \equiv [V]_E,$$

and shall write $[V]_E(i, j)$ for the entry at subscripts (i, j). If the base(s) are clear from the context, we shall simply write $M(V)$ and v_{ij}, respectively.

For the basics on cardinal numbers we refer the reader, e.g., to Kuratowski and Mostowski [K-M].

2. The results

We shall need the following simple lemma, which shows that nonnegative unitary operators in the infinite-dimensional Hilbert space case are natural generalizations of permutation operators (matrices) in the finite-dimensional case.

Lemma 1. *If V is an (E, F)-nonnegative isometry, then its matrix $M(V; E, F)$ has in each row at most one positive entry, and has in each column at least one positive entry. If V^* is an (F, E)-nonnegative isometry, then $M(V; E, F)$ has in each column at most one positive entry, and has in each row at least one positive entry. A consequence: V is an (E, F)-nonnegative unitary operator if and only if the infinite matrix $M(V; E, F)$ contains exactly one entry 1 in each row and in each column; all other entries are 0.*

Proof. If V is an (E, F)-nonnegative isometry, we have

$$\sum_j v_{ji} v_{jk} = (Ve_i, Ve_k) = (e_i, e_k) = \delta_{ik}.$$

Since all entries are nonnegative, if $v_{ji} > 0$, then all the other entries in row j must be 0. Furthermore, for each i we have $\sum_j v_{ji}^2 = 1$. Hence there is a positive entry in each column.

The matrix of the adjoint V^* with respect to the bases (F, E) is the conjugate transpose of the matrix $M(V; E, F)$. Hence, if V^* is an isometry, there is a positive entry in each row, and at most one positive entry in each column of $M(V; E, F)$.

As a consequence, if V is unitary, there is exactly one positive entry in each row and each column in the matrix of V. Furthermore, we see that this entry must equal 1. Conversely, if there is exactly one entry 1 in each row and each column in the matrix of V, then V induces a bijection of the orthonormal basis E onto the orthonormal basis F. Hence V is clearly unitary and also (E, F)-nonnegative. □

Remark. Note that if V is any unitary operator and $F := V(E)$, then V is (E, F)-nonnegative.

With the notation above consider an arbitrary (E, E)-nonnegative unitary operator $U : H \to H$. The first result of this paper establishes a (nonnegative) canonical form, depending on E, for U that will provide a complete set of unitary invariants. In order to be able to formulate the theorem, we introduce the following notation. The identity operator and matrix in any Hilbert space will be denoted by I, and in n-dimensional Hilbert space the operator S_n $(n \geq 2)$ will have (with respect to the given orthonormal basis B) the matrix representation

$$M(S_n; B, B) = \begin{pmatrix} 0 & 0 & \dots & 0 & 1 \\ 1 & 0 & \dots & 0 & 0 \\ 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & 0 \end{pmatrix}.$$

The bilateral shift operator of multiplicity 1 in the space $l^2(\mathbf{Z})$ will be denoted by S, and will have in the given orthonormal basis the infinite matrix representation containing 1 immediately below the main diagonal and 0 everywhere else. With this notation we formulate our first result as follows, and refer for the basic graph-theoretic notions used in the proof, e.g., to the monograph [Kon] by D. König.

Theorem 1. *Let $U : H \to H$ be an (E, E)-nonnegative unitary operator. Then there is a Hilbert space K with an orthonormal basis F and an (F, E)-nonnegative unitary operator $V : K \to H$ such that V^{-1} is (E, F)-nonnegative unitary, and*

$$(*) \qquad V^{-1}UV = I \oplus (S_2 \oplus S_2 \oplus \cdots) \oplus (S_3 \oplus S_3 \oplus \cdots) \oplus \cdots \oplus (S \oplus S \oplus \cdots).$$

Let $d(1) \equiv d(1, E)$ denote the (orthogonal) dimension of the Hilbert space of the operator I, let $d(n) \equiv d(n, E)$ denote the cardinality of the terms in the nth orthogonal summand $(\cdot)$, and let $d(\infty) \equiv d(\infty, E)$ denote the cardinality of the terms in the last orthogonal summand $(\cdot)$. The sequence of cardinalities

$$d(U, E) := \{d(\infty), d(1), d(2), d(3), \dots\}$$

is uniquely determined by E, and may depend on the considered basis E.

For each $j \in \mathbf{N}$ define the cardinal

$$c(j) \equiv c(j, E) := \sum \{d(jr) : r \in \mathbf{N}\}.$$

(For the cardinality $\aleph_0$ we shall also write ∞ in what follows.) Furthermore, define $c(\infty) := d(\infty)$ and

$$c(U) \equiv c(U, E) := \{c(\infty), c(1), c(2), c(3), \dots\}.$$

Then the sequence of cardinalities c does not depend on E. If B is any orthonormal basis in H for which U is (B, B)-nonnegative, then the corresponding sequence c of cardinalities is again $c(U)$. Furthermore, the sequence $c(U)$ is a complete set of unitary invariants for U in the following sense: assume that A is a bounded linear operator in a Hilbert space Q. A is unitarily equivalent to U if and only if for some orthonormal basis R in Q the operator A is (R, R)-nonnegative unitary and $c(A) = c(U)$.

Proof. Lemma 1 shows that the infinite matrix of U with respect to the bases (E, E) has exactly one 1 in each row and in each column; all other entries are 0. Define the corresponding directed graph $D = D(U, E)$ as follows. The vertices of D are the elements of E or, equivalently, the corresponding indices, and the ordered pair (p, q) is an edge if and only if $u_{pq} = 1$. The corresponding non-directed graph will be denoted by $G = G(U, E)$. The (in general, infinite) graph G has the property that each vertex is the endpoint of at most two edges. Hence [Kon, Satz 27, Kap. I, p. 17] applies and shows that each connected component of G is either a path or a cycle or a unilateral infinite path or a bilateral infinite path. Furthermore, Sätze 21-23 there show that the graph G is the graph-theoretic sum of its uniquely determined connected components, and that if p and q are vertices belonging to different connected components, then there is no path connecting the two vertices.

Assume that there is a connected component G_a in the graph G which is a path, say $p_1p_2\dots p_n$. Then either the pair (p_1,p_2) or (p_2,p_1) is an edge in D. To consider a definite case, assume that $u_{p_1p_2}=1$. In view of the 0-1 pattern of the matrix $M(U)$ of U we then have $u_{p_1p_2}\dots u_{p_{n-1}p_n}=1$. The pattern of $M(U)$ shows, however, that there is an index j such that $u_{jp_1}=1$. This contradicts the maximality of the connected component path above. Hence there cannot be such a connected component. Assuming the existence of a connected component G_b which is a unilateral infinite path $p_1p_2\dots$, we reach a contradiction in a similar way. Hence each connected component of G is either a cycle or a bilateral infinite path (cf. also Ore [O, pp. 25–27]).

Assume that the cardinality of the set of the row (or, equivalently, column) indices k_j such that $u_{k_jk_j}=1$ is $d(1)$, and let K_1 be a Hilbert space with an orthonormal basis F_1 of the same cardinality. For any $f_j\in F_1$ define $V_1f_j:=e_{k_j}$. Then $V_1^{-1}UV_1$ clearly extends to the identity on K_1.

Consider now a connected component G_a that is a cycle of n vertices, say $p_1p_2\dots p_np_1$. Similarly, as in the penultimate paragraph, we establish that there are two possibilities: in order to consider a definite case we may and shall assume that $u_{p_1p_n}=\dots=u_{p_2p_1}=1$. This means for the corresponding basis vectors in E that

$$Ue_{p_1}=e_{p_2},\dots,Ue_{p_n}=e_{p_1}.$$

Taking the n-dimensional Hilbert space $\mathbf{C}^n$ with orthonormal basis $\{b_1,\dots,b_n\}$ and defining $W_nb_j:=e_{p_j}$, we obtain that $W_n^{-1}UW_n$ extends to S_n. Forming the orthogonal sum K_n of $d(n)$ copies of $\mathbf{C}^n$, the union F_n of the corresponding orthonormal bases and the corresponding orthogonal sum $V_n=W_n\oplus W_n\oplus\dots$, we have in the space K_n,

$$V_n^{-1}UV_n=S_n\oplus S_n\oplus\dots.$$

Consider now a connected component G_a that is a bilateral infinite path, say $\dots,q_{-1},q_0,q_1,\dots$. Considering again one of two possibilities, assume that $u_{q_jq_{j+1}}=1$ for every $j\in\mathbf{Z}$. Take the canonical orthonormal basis $\{b_j;j\in\mathbf{Z}\}$ in $l^2(\mathbf{Z})$, and define $Wb_j:=e_{q_{-j}}$. Then $W^{-1}UWb_j=b_{j+1}$ for every $j\in\mathbf{Z}$, i.e., $W^{-1}UW$ extends to S. Forming the orthogonal sum K_∞ of $d(\infty)$ copies of $l^2(\mathbf{Z})$, the union F_∞ of the corresponding orthonormal bases, and the orthogonal sum V_∞ of the corresponding operators, we have in the space K_∞,

$$V_\infty^{-1}UV_\infty=S\oplus S\oplus\dots.$$

Forming again the required orthogonal sums, e.g.,

$$V:=V_1\oplus V_2\oplus\dots\oplus V_\infty,$$

we clearly obtain the first statement of the theorem. Furthermore, the construction shows that the considered basis E uniquely determines the sequence of cardinals $d(U,E)$.

Assume now that U is also (B,B)-nonnegative unitary for some orthonormal basis B in H. Then U is also unitary equivalent to a representation of the form $(*)$, where the sequence of cardinals $d(U,B)$ may naturally depend on B. The representations for E and B are unitarily equivalent. So we shall seek a convenient form for a complete set of unitary invariants for representations of the form $(*)$. A complete set of unitary invariants is naturally given by the multiplicity theory for normal operators. For the general theory in nonseparable Hilbert spaces we refer the reader to [Hal1] or [Bro] or [Ples], and we shall cite the relevant and needed facts without detailed reference.

It is well known (see, e.g., [Conw]) that each summand S is unitarily equivalent to the multiplication operator N_q by the identity function on the space $L \equiv L^2(C_1, q)$, where C_1 is the unit circle in $\mathbf{C}$ and q is normalized Lebesgue measure on C_1. Hence we may and shall replace in each representation $(*)$ the operators S by the operators N_q.

For uniformity in the notation write S_1 for the 1-dimensional identity operator (or matrix), and consider a representation in the space H of the form

$$T := (S_1 \oplus S_1 \oplus \cdots) \oplus (S_2 \oplus S_2 \oplus \cdots) \oplus (S_3 \oplus S_3 \oplus \cdots) \oplus \cdots \oplus (N_q \oplus N_q \oplus \cdots),$$

where the sequence of cardinals d is now determined by the basis B. It is clear that the operator T is the orthogonal sum of its "point part" T_p, which is the orthogonal sum of all the parts denoted above by S_k, and of its absolutely continuous part T_a (with respect to Lebesgue measure on the unit circle C_1), which is the orthogonal sum of all the parts N_q. A complete system of unitary invariants (in our case) can be given by the union of a complete system for T_p and of a complete system for T_a. The latter part clearly has the spectral type (in Plesner's terminology) $d(\infty, B)m \equiv c(\infty, B)m$, where m is the spectral type of the Lebesgue measure above. Hence the cardinal $c(\infty) \equiv c(\infty, B)$ is a complete system for the part T_a.

It is known that a complete system for the point part T_p is given by the multiplicities (in the generally used terminology) of the numbers in the point spectrum of the operator T_p. This point spectrum is the union of the point spectra of all the (occurring) parts S_k. So it is a subset of the set

$$\sigma := \{e^{2\pi i r/n} : n \in \mathbf{N}, r = 1, 2, \ldots, n\}.$$

For a fixed value $n \in \mathbf{N}$ the number $e^{2\pi i/n}$ can only appear in the (point) spectra of S_{nr}, $r \in \mathbf{N}$, with multiplicity 1. Hence its multiplicity in the part T_p is

$$\mu(e^{2\pi i/n}) = \sum_{r \in \mathbf{N}} d(nr, B) = c(n, B).$$

Furthermore, if the positive integers k, n are relatively prime, then clearly

$$\mu(e^{2\pi i k/n}) = \mu(e^{2\pi i/n}) = c(n, B).$$

Hence the multiplicity of each number in the point spectrum of T_p is determined by the corresponding term in the sequence of cardinals $\{c(1, B), c(2, B), \ldots\}$. Conversely, the multiplicities determine the sequence c. Therefore, the whole sequence $\{c\}$ of cardinals is independent of the basis B, and is a complete system of unitary invariants for $T = T_p \oplus T_a$.

Now let A be a bounded linear operator in a Hilbert space Q. Assume first that A is (R, R)-nonnegative unitary for some orthonormal basis R in Q, and that $c(A) = c(U)$. By what has been proved above, A is unitarily equivalent to U. Conversely, assume that to the operator A there exists a unitary $T : Q \to H$ satisfying $A = T^{-1}UT$. Let $R := T^{-1}(E)$. Then R is an orthonormal basis in Q, and A is clearly (R, R)-nonnegative unitary. With the notation $Tr_j = e_j$ for all indices, the unitary equivalence above shows that the corresponding matrices in the bases R and E, respectively, have identical entries for every pair of indices i, j:

$$[A]_R(i,j) = (Ar_j, r_i) = (T^*UTr_j, r_i) = (Ue_j, e_i) = [U]_E(i,j).$$

The equality of the matrices above (in the corresponding bases) yields that the cardinalities of the sets of the cycles of equal lengths are equal. Hence $d(A,R) = d(U,E)$, which implies $c(A) = c(U)$. The proof is complete. ☐

Remark. It is clear that the Hilbert space K in the statement can also be chosen to be H, and the basis F can be a permutation of E. Furthermore, simple examples show that the sequence d is, in general, not a set of unitary invariants. For example, the operators

$$U_1 := S_1 \oplus S_2 \oplus S_3 \oplus \dots, \qquad U_2 := U_1 \oplus U_1$$

are, by Theorem 1, unitarily equivalent, since for both we have

$$c(1) = c(2) = \cdots = \infty.$$

On the other hand, the sequences d are different.

Remark. Let $U : H \to H$ be an (E,E)-nonnegative unitary operator. Then U is unitarily equivalent to its adjoint U^*, and $d(U^*, E) = d(U, E)$.

Corollary. *Let $U : H \to H$ be an (E,E)-nonnegative unitary operator. Then the point spectrum of U is the set*

$$\bigcup \{J(n) : n \in \mathbf{N}, d(n,E) > 0\},$$

where $J(n)$ denotes the set of the nth roots of unity, and $d(n,E)$ is the corresponding element of $d(U,E)$.

Proof. The point spectrum of any orthogonal sum of operators is the union of the point spectra of the operators. Since the point spectrum of the bilateral shift is empty, the canonical decomposition of Theorem 1 yields the statement. ☐

Remark. If H is finite-dimensional, this Corollary gives the spectrum of U.

Theorem 2. *The unitary operator U is nonnegative with respect to some orthonormal basis E if and only if for its canonical decomposition into singular continuous, absolutely continuous (w.r.t. Lebesgue measure) and point parts*

$$U = U_s \oplus U_a \oplus U_p$$

the following conditions hold: the subspace H_s of U_s is $\{0\}$, the spectral type of the part U_a is cm, where c is any cardinal and m is the spectral type of Lebesgue measure on C_1, the point spectrum of the operator U_p is a subset of the set

$$\sigma := \{e^{2\pi i r/n} : n \in \mathbf{N}, r = 1, 2, \dots, n\},$$

and if the cardinal c_n denotes the multiplicity of the number $e^{2\pi i/n}$ (in the point spectrum, in the usual sense) for U (or, equivalently, for U_p), then:

1) *$j|n$ (i.e., j divides n) implies $c_j \geq c_n$.*

2) *If c_n is a finite cardinal, then there is a nonnegative integer r_n such that for every $r > r_n$ we have $c_{nr} = 0$, and*

$$c_n + \sum_{p_2} c_{np_2} + \sum_{p_4} c_{np_4} + \cdots \geq \sum_{p_1} c_{np_1} + \sum_{p_3} c_{np_3} + \dots.$$

(*In the above formula, p_k means any product of k pairwise distinct primes, and summation is extended to all such products. The conditions clearly imply that all* *sums above contain only a finite number of nonzero terms; hence we have simple additions on both sides.*)

3) *If k, n are relatively prime, then, for the multiplicities,*

$$\mu(e^{2\pi ik/n}) = \mu(e^{2\pi i/n}) = c_n.$$

Proof. Necessity. Assume that U is nonnegative unitary with respect to some orthonormal basis E. Theorem 1 shows that then the first conditions and 3) hold, and

$$c_n = c(n) = \sum_{r\in\mathbf{N}} d(nr, E). \tag{+}$$

We shall show that 1) and 2) are also satisfied.

If $j|n$, then there is $s \in \mathbf{N}$ such that $n = js$. Hence

$$c_n = \sum_{r\in\mathbf{N}} d(nr) = \sum_{r\in\mathbf{N}} d(jsr) \leq \sum_{r\in\mathbf{N}} d(jr) = c_j;$$

so 1) holds.

If c_n is a finite cardinal, then (+) shows that there is r_n such that $r > r_n$ implies $d(nr) = 0$. On the other hand, this implies that $c_{nr} = 0$, as stated. The connection between the relevant nonnegative integer numbers d and c is then the following finite system of linear equations:

$$\begin{aligned}
d(n) + d(2n) + d(3n) + d(4n) + d(5n) + d(6n) + \cdots + d(r_n n) &= c_n \\
d(2n) + d(4n) + d(6n) + \cdots + \ldots &= c_{2n} \\
d(3n) + d(6n) + \cdots + \ldots &= c_{3n} \\
\cdots + \cdots + \ldots &= \ldots \\
d(r_n n) &= c_{r_n n}.
\end{aligned} \tag{$**$}$$

The structure of this system shows that, in the notation of the theorem, $d(n)$ can be written as

$$d(n) = c_n - \sum_{p_1} c_{np_1} + \sum_{p_2} c_{np_2} - \sum_{p_3} c_{np_3} + \sum_{p_4} c_{np_4} + \ldots, \tag{$+-$}$$

where the stated finiteness of all the sums clearly holds. Indeed, let us check that the summation on the right-hand side of $(+-)$ leaves only $d(n)$ from the left-hand side of the equations $(**)$: if $d(qn)$ $(q \geq 2)$ occurs on the left-hand side of $(**)$, and we have the prime factorization $q = q_1^{a_1} \ldots q_s^{a_s}$ with pairwise distinct factors $q_1, \ldots, q_s$, then the coefficient of $d(qn)$ on the right-hand side of $(+-)$ is

$$\binom{s}{0} - \binom{s}{1} + \binom{s}{2} - \cdots = (1-1)^s = 0.$$

Since each $d(n) \geq 0$, we obtain the stated inequality in 2).

Sufficiency. The assumption on the spectral type of the part U_a implies that U_a is unitarily equivalent to the orthogonal sum of c copies of the operator N_q or, equivalently, of the operator S. The part U_s is clearly 0. The point spectrum of the "point part" U_p is contained in the set σ above, and the sequence $\{c_n : n \in \mathbf{N}\}$ of cardinals, by condition 3), determines uniquely the multiplicity of each point in the point spectrum of U_p (or, equivalently, of U). Using conditions 1) and 2), we shall show that we can determine a (not necessarily unique) sequence $\{d(n) : n \in \mathbf{N}\}$ of cardinals such that U_p is unitarily equivalent to the orthogonal sum of the sums of $d(n)$ copies of the operator S_n $(n = 1, 2, \dots)$.

If for a fixed $n \in \mathbf{N}$ the cardinal c_n is finite, then we *define* the integer $d(n)$ by the equation $(+-)$. By condition 2), $d(n)$ is then a nonnegative integer. By condition 1), then

$$\infty > c_n \geq c_{2n} \geq \dots \geq c_{r_n n}.$$

Hence we can and shall define $d(2n), d(3n), \dots, d(r_n n)$ similarly. Therefore, the finite sequence

$$\{d(n), d(2n), \dots, d(r_n n)\}$$

is the unique solution of the linear system of equations $(**)$. It follows that

$$\sum_{r \in \mathbf{N}} d(rn) = \sum_{r=1}^{r_n} d(rn) = c_n.$$

If for a fixed n the cardinal c_n is infinite, then we define $d(n) := c_n$. Then, clearly,

$$\sum_{r \in \mathbf{N}} d(rn) \geq c_n.$$

On the other hand, applying these definitions of $d(\cdot)$ and 1), for every $r \in \mathbf{N}$ we obtain the following inequality for the cardinals:

$$d(rn) \leq c_{rn} \leq c_n.$$

Hence

$$\sum_{r \in \mathbf{N}} d(rn) \leq \sum_{r \in \mathbf{N}} c_n \leq c_n \aleph_0 \leq c_n c_n = c_n.$$

We have obtained for every $n \in \mathbf{N}$,

$$\sum_{r \in \mathbf{N}} d(rn) = c_n.$$

By Theorem 1, the operator

$$T := (S_1 \oplus S_1 \oplus \dots) \oplus (S_2 \oplus S_2 \oplus \dots) \oplus \dots$$

with $d(1), d(2), \dots$ copies of orthogonal summands in each term in parentheses is then unitarily equivalent to the operator U_p (which has the point spectrum multiplicities c_n). Hence

$$V := (S \oplus S \oplus \dots) \oplus T$$

(with c copies of S in the parentheses) is unitarily equivalent to U. Since V is clearly nonnegative unitary with respect to some orthonormal basis B, by Theorem 1, U is nonnegative unitary for an orthonormal basis E. The proof is complete. $\square$

Example. The following classical example will demonstrate the applicability of Theorem 2.

Consider the Fourier-Plancherel operator U in the space $H := L^2(\mathbf{R})$, i.e., let

$$(Ug)(y) := (2\pi)^{-1/2} \int_{\mathbf{R}} g(x) e^{ixy} dx \qquad (g \in L^2(\mathbf{R})),$$

where the integral is understood in the well-known sense. It is known that the normalized Hermite functions f_n $(n = 0, 1, 2, \dots)$ defined by

$$f_n(x) := (-1)^n (2^n n! \sqrt{\pi})^{-1/2} e^{x^2/2} (\frac{d}{dx})^n e^{-x^2}$$

form an orthonormal basis F in the separable space H. Furthermore, for every n we have $Uf_n = i^n f_n$. It is also known (see, e.g., [R:Sz-N]) that the operator U is unitary with spectrum $\{1, i, -1, -i\}$. Hence the ranges of the corresponding spectral projections are the respective spanned closed linear subspaces

$$P(U, i^k)H = \overline{sp}\{f_{k+4n}; n = 0, 1, 2, \dots\} \qquad (k = 0, 1, 2, 3).$$

We see that the multiplicities of the points i^k in the (point) spectrum (i.e., the orthogonal dimensions of the subspaces) are all $\aleph_0$. Hence the conditions 1), 2), and 3) in Theorem 2 are satisfied:

$$c_1 = c_2 = c_4 = \aleph_0, \quad \mu(e^{2\pi i 3/4}) = \aleph_0 = c_4,$$

and $c_k = 0$ for every other positive integer k. By Theorem 2, there is an orthonormal basis E such that $M(U; E, E)$ is nonnegative. We shall show (what is clear from the corresponding part of the proof), that also in our case the sequence d is not determined uniquely. For example, define the vector $e_{4n} \in H$ with the help of the vectors f_{4n+k} $(k = 0, 1, 2, 3)$ for every $n = 0, 1, 2, \dots$ in the same way as for the case $n = 0$:

$$\begin{aligned} e_0 &:= \frac{1}{2}(f_0 + f_1 + f_2 + f_3), \\ e_1 &:= Ue_0 = \frac{1}{2}(f_0 + if_1 - f_2 - if_3), \\ e_2 &:= Ue_1 = \frac{1}{2}(f_0 - f_1 + f_2 - f_3), \\ e_3 &:= Ue_2 = \frac{1}{2}(f_0 - if_1 - f_2 + if_3). \end{aligned}$$

Then we have defined 4 vectors such that $\{e_0, e_1, e_2, e_3\}$ is another orthonormal basis for the subspace spanned by the corresponding vectors f and, in addition to the indicated mapping properties, $Ue_3 = e_0$. Continuing in exactly the same way in each corresponding 4-dimensional subspace, we obtain the orthonormal basis E, with respect to which $M(U; E, E)$ is nonnegative, $d(4, E) = \aleph_0$, and every other $d(k, E) = 0$.

It is now also clear how we can obtain an orthonormal basis B, for which $M(U; B, B)$ is nonnegative, and (as in the proof of Theorem 2)

$$d(1, B) = d(2, B) = d(4, B) = \aleph_0,$$

and every other $d(k, B) = 0$. To begin, define

$$\begin{aligned} &b_0 := f_0,\ b_1 := \frac{1}{\sqrt{2}}(f_4 + f_2),\ b_2 := \frac{1}{\sqrt{2}}(f_4 - f_2), \\ &b_3 := \frac{1}{2}(f_8 + f_1 + f_6 + f_3),\ b_4 := \frac{1}{2}(f_8 + if_1 - f_6 - if_3), \\ &b_5 := \frac{1}{2}(f_8 - f_1 + f_6 - f_3),\ b_6 := \frac{1}{2}(f_8 - if_1 - f_6 + if_3), \end{aligned}$$

and continue in this way in the appropriate 7-dimensional subspaces. The constructed basis B will satisfy all the requirements.

The next result (the case of a finite-dimensional space) would follow from Theorems 1 and 2. However, we prefer another proof, showing the usefulness of the trace in this situation.

Theorem 3. *Let U be an (E,E)-nonnegative unitary operator in the finite-dimensional Hilbert space $H = \mathbf{C}^N$. Consider the finite sequence of nonnegative numbers*

$$d(U) \equiv d(U,E) := \{d(1,E), d(2,E), d(3,E), \dots, d(u,E)\},$$

where the cardinals $d(k,E)$ $(1 \le k \le u < \infty)$ have the same meaning as in Theorem 1 (and are now finite). Then the sequence $d(U,E)$ does not depend on E, and is a complete set of unitary invariants for U in the following sense: assume that A is a bounded linear operator in a Hilbert space Q. A is unitarily equivalent to U if and only if for some orthonormal basis R in Q the operator A is (R,R)-nonnegative unitary, and $d(A,R) = d(U,E)$.

Proof. Assume first that U is also (B,B)-nonnegative unitary for some orthonormal basis B in H. Denote the corresponding basis elements by e_j, b_j $(j = 1, \dots, N)$, respectively, define $We_j := b_j$, and extend it in the obvious way to H. Then W is a unitary operator and, by assumption,

$$(W^*UWe_i, e_j) = (UWe_i, We_j) = (Ub_i, b_j) \ge 0$$

for all subscripts i, j. Denoting the matrix of U in the basis B by $[U]_B$, we obtain for every $k \in \mathbf{N}$,

$$[U]_B^k = [W^*UW]_E^k = [W^*]_E [U]_E^k [W]_E.$$

Hence the traces of $[U]_B^k$ and $[U]_E^k$ are equal, and both matrices are clearly permutation matrices. By Theorem 1, the first powers are unitarily equivalent to matrices of the form

$$M_E = (M(S_1) \oplus \cdots \oplus M(S_1)) \oplus (M(S_2) \oplus \cdots \oplus M(S_2)) \oplus \cdots \oplus (M(S_u) \oplus \cdots \oplus M(S_u)),$$

where all matrices $M(S_k)$ are now $M(S_k; E, E)$ for $2 \le k \le u$, and $M(S_1) \oplus \cdots \oplus M(S_1)$ is the $d(1,E)$-dimensional identity matrix (and everything similarly for the basis B). Furthermore, the numbers of the summands in the consecutive parentheses are $d(1,E), d(2,E), \dots, d(u,E)$, and similarly for the basis B. Hence, with self-explaining notation,

$$d(1,B) = \mathrm{trace}(M_B) = \mathrm{trace}(M_E) = d(1,E) =: d(1),$$

$$d(1) + 2d(2,B) = \mathrm{trace}(M_B^2) = \mathrm{trace}(M_E^2) = d(1) + 2d(2,E).$$

Hence $d(2,B) = d(2,E) =: d(2)$. Furthermore,

$$d(1) + 3d(3,B) = \mathrm{trace}(M_B^3) = \mathrm{trace}(M_E^3) = d(1) + 3d(3,E).$$

Continuing in this way, we obtain that

$$d(U,E) = d(U,B) \tag{++}$$

is independent of the bases as stated.

The last sentence in the statement of the theorem is proved exactly as in the proof of Theorem 1. Since in the finite-dimensional case we have (++), we obtain that A is unitarily equivalent to U if and only if $d(A) = d(U)$, independently of the bases. Hence we have proved that the finite sequence $d(U)$ is a complete set of unitary invariants in the sense stated in the theorem. □

For the basic facts on the von Neumann-Wold decomposition of isometries see, e.g., [Sz-N:F] or [Hal2].

Theorem 4. *Assume that $V : H \to H$ is an isometry with unitary part V_u. V_u is nonnegative for some orthonormal basis F in its subspace H_u if and only if there is an orthonormal basis E in H such that the matrix $M(V; E, E)$ has exactly one* 1 *in each column* (*all other entries in the column are* 0). *In this case the cardinal of the set of the zero rows is the multiplicity of the unilateral shift part V_t in the Wold decomposition.*

Proof. Assume first that the matrix $M(V_u; F, F)$ is nonnegative. By Lemma 1, it has then exactly one 1 in each row and in each column; all other entries are 0. It is well known that each isometry, hence V, is the orthogonal sum of its unitary part V_u and of a (multiple, unilateral) shift V_t. The latter is, in turn, the orthogonal sum (of some cardinality) of simple (unilateral) shifts T, which have for some orthonormal basis B of cardinality $\aleph_0$ the infinite matrix $M(T; B, B)$ having 1's immediately below the main diagonal and 0's everywhere else, i.e., satisfying

$$Tb_k = b_{k+1} \qquad (b_k \in B,\ k = 1, 2, \dots).$$

Taking the union of the bases F and B, from the latter one of the cardinality determined by the orthogonal sum (i.e., by the multiplicity of the multiple shift), we obtain an orthonormal basis E that satisfies the requirements of the necessity statement.

Assume now that each column in $M(V; E, E)$ has exactly one entry 1 and all other entries in the column are 0. Then the subspace $V(H)$ consists exactly of the vectors $h \in H$, the components of which corresponding to the zero rows of the matrix are 0. The "canonical" wandering subspace H_w for V is the orthogonal complement of $V(H)$. Hence an orthonormal basis E_w for it consists of all the vectors $e_j \in E$ corresponding to the zero rows in the matrix. The subspace H_t of the unilateral shift part V_t is the orthogonal sum of the subspaces $V^n H_w$ for $n = 0, 1, 2, \dots$. Hence the set $S := \bigcup_{n=0}^{\infty} V^n E_w$ is an orthonormal basis for H_t. The 0-1 structure of the matrix shows that each vector $V^n e_j \in V^n E_w$ is again a vector in the basis E; hence $S \subseteq E$. From this, $S = E \cap H_t =: E_t$. The (in general, infinite) submatrix of $M(V; E, E)$ based on the subset $E_u := E \setminus E_t$ of E has exactly one 1 in each column and in each row; all other entries are 0. Hence it is the matrix of an (E_u, E_u)-nonnegative unitary operator, which is the unitary part V_u of V in the canonical (Wold) decomposition. The construction shows also that the cardinal of the zero rows in $M(V; E, E)$ is exactly the multiplicity of the multiple shift V_t in the Wold decomposition. □

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