

Positive elements in the algebra of the quantum moment problem[★]

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Summary. Let \mathfrak{A} denote the extended Weyl algebra, $\mathfrak{A}_0 \subset \mathfrak{A}$, the Weyl algebra. It is well known that every element of \mathfrak{A} of the form $A = \sum B_k^* B_k$ is positive. We prove that the converse implication also holds: Every positive element A in \mathfrak{A} has a quadratic sum factorization for some finite set of elements (B_k) in \mathfrak{A} . The corresponding result is not true for the subalgebra \mathfrak{A}_0 . We identify states on \mathfrak{A}_0 which do not extend to states on \mathfrak{A} . It follows from a result of Powers (and Arveson) that such states on \mathfrak{A}_0 cannot be completely positive. Our theorem is based on a certain regularity property for the representations which are generated by states on \mathfrak{A} , and this property is not in general shared by representations generated by states defined only on the subalgebra \mathfrak{A}_0 .

0. Introduction

For the moment problem in several variables, we consider linear functionals ω on the polynomials \mathcal{P} such that $\omega(\bar{p}p) \geq 0$ for all $p \in \mathcal{P}$. It is known, from general theory (see [Fu] for references), that this condition on ω is strictly weaker than the condition, $\omega(q) \geq 0$ for all $q \in \mathcal{P}$ such that $q \geq 0$ pointwise in \mathbb{R}^n . For $n = 1$ they are equivalent. Note that for $n \geq 2$, not every $q \geq 0$ can be written as a finite (polynomial) sum, $q = \sum \bar{p}p$. (See [Fu] and [Sc1].) In this paper, we shall be concerned with positivity in non-abelian algebras which are analogous to \mathcal{P} . These algebras are generated by variables x_1, \dots, x_n , now subject to certain relations to be specified. In case of the canonical commutation relations, we have the associated quantum problem of moments, reconstructing a positive functional on the so called Weyl algebra [Di] as a non-commutative integral against an operator valued measure (whenever possible). An element in the Weyl algebra is said to be positive if it defines a positive semidefinite quadratic form in the Schrödinger representation. While positive elements in the Weyl algebra cannot generally be expressed as finite sums $\sum H^*H$ for elements H in the algebra, we show that such a representation

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does hold for all positive elements in a certain extension of the Weyl algebra. The individual elements H from the sum will then again be in the extended algebra. This problem arose from our desire to expand the spectral resolution of quantum mechanical operators in terms of algebraic conditions, in a manner which is analogous to the usual eigenfunction expansion of the number-operator for Bosons.

1. The extended Weyl algebra

The algebra \mathcal{W} with unit 1, generators x , p , and relation

$$xp - px = \sqrt{-1}1 \quad (1.1)$$

is called the Weyl algebra. Let $i = \sqrt{-1}$, and let $\tilde{\mathcal{W}}$ be the algebra over the same commutation relation, but now with generators, x , p and $(ax + i1)^{-1}$ for $a \in \mathbb{R}$. We shall call $\tilde{\mathcal{W}}$ the extended Weyl algebra.

For the extended Weyl algebra $\tilde{\mathcal{W}}$, we have the further pair of relations on the generators,

$$[p, (ax + i1)^{-1}] = ia(ax + i1)^{-2} \quad \text{for all } a \in \mathbb{R},$$

where $[\cdot, \cdot]$ denotes the commutator bracket. These must be added to the Heisenberg commutation relation (1.1) above defining \mathcal{W} . Of course, we have the relations

$$(x \pm i1)^{-1}(x \pm i1) = 1 = (x \pm i1)(x \pm i1)^{-1}$$

which are implicit in the notation, and will be used without mention. Both algebras, \mathcal{W} and $\tilde{\mathcal{W}}$, may be realized on $L^2(\mathbb{R}) =$ (all square-integrable functions on the real line) in the Schrödinger representation σ . In this representation, the operator $\sigma(x)$ becomes multiplication by the variable x , i.e., the quantum mechanical position operator, and $\sigma(p)$ becomes the corresponding momentum operator, viz., $-i \frac{d}{dx}$.

For elements h in $\tilde{\mathcal{W}}$, the corresponding operator will be denoted with capitals, e.g., $H = \sigma(h)$. We shall further use the notation, $\mathfrak{A}_0 = \sigma(\mathcal{W})$, and $\mathfrak{A} = \sigma(\tilde{\mathcal{W}})$. Note that \mathfrak{A} is an algebra of operators on $L^2(\mathbb{R})$. The elements in \mathfrak{A} are (generally) unbounded operators. For A in \mathfrak{A} , A^* denotes the adjoint operator where the adjoint star is defined relative to the $L^2(\mathbb{R})$ -inner product, i.e.,

$$\langle Af, g \rangle = \langle f, A^*g \rangle, \quad A \in \mathfrak{A}, f, g \in \mathcal{S}$$

where \mathcal{S} denotes the Schwartz space of functions on \mathbb{R} , and where

$$\langle f, g \rangle = \int_{-\infty}^{\infty} \overline{f(x)}g(x)dx.$$

Note that $A^* \in \mathfrak{A}$, so \mathfrak{A} acquires the structure of a Hermitian algebra where the $*$ -involution is the above mentioned operator adjoint.

Let

$$A = 2^{-\frac{1}{2}}(X + iP), \quad \text{and} \quad N = A^*A. \quad (1.2)$$

These are the quantum mechanical annihilation operator, respectively number operator; and it is well known that the spectrum of N is $\{0, 1, 2, \dots\}$. It follows that the operator

$$T = (N - I)(N - 2I) \tag{1.3}$$

satisfies $\langle f, Tf \rangle \geq 0$. However, T is *not* a finite sum of operators of the form H^*H for $H \in \mathfrak{A}_0$. This was noted in [Wo], but can also be verified by direct inspection. We prove, in Sect. 6 below, that T may be factored as $T = C^*C$ for C in the extended algebra \mathfrak{A} .

2. Spectrum from algebra

The present paper arose from a desire to determine the spectrum of elements in \mathfrak{A} from a suitable set of algebraic conditions, similar to the conditions which dictate the spectrum of the harmonic oscillator Hamiltonian N , i.e., the well known algebraic realization of the Hermite functions in $L^2(\mathbb{R})$ as eigenfunctions of N . In standard quantum mechanics books, e.g., [PW], the eigenfunctions are obtained by normalization of the vector sequence $A^{*n}f_0$ where $f_0(x) = e^{-\frac{1}{2}x^2}$. Recall the familiar commutator formula

$$[N, A^{*n}] = nA^{*n} \tag{2.1}$$

which is based on the canonical commutation relation, written in the form

$$[A, A^*] = AA^* - A^*A = I. \tag{2.2}$$

A linear functional ω on \mathfrak{A}_0 is called a *state* if

$$\omega(I) = 1, \text{ and } \omega(H^*H) \geq 0, \text{ } H \in \mathfrak{A}_0. \tag{2.3}$$

It is well known (see e.g., [Po] in the present context) that the GNS-representation applies to states ω on \mathfrak{A}_0 ; and each ω generates a Hermitian representation $\pi = \pi_\omega$ of \mathfrak{A}_0 on a Hilbert space \mathcal{H}_ω with cyclic vector $\Omega = \Omega_\omega$ such that

$$\omega(A) = \langle \Omega, \pi(A)\Omega \rangle, \text{ } A \in \mathfrak{A}_0 \tag{2.4}$$

where $\langle \cdot, \cdot \rangle$ refers to the inner product in \mathcal{H}_ω . Note also that the normalization, $\omega(I) = 1$, corresponds to, $\|\Omega\| = 1$. The Hermitian property of π is given by the identity, $\langle \pi(H)\psi_1, \psi_2 \rangle = \langle \psi_1, \pi(H^*)\psi_2 \rangle$, $H \in \mathfrak{A}_0$, $\psi_1, \psi_2 \in \mathcal{S}$.

The element T , given by (1.3), was used by Woronowicz [Wo1] to illustrate “singularities” for the “quantum problem of moments”: Specifically, to give an example of a non-normal state on the Weyl algebra. There are familiar, and analogous singularities for the classical moment problem in two (commuting) variables arising from the known positive two-variable polynomials which cannot be written as (finite) sum of “squares”, see e.g., [Fu], [Sc1], [Po] and [Wo1–2].

In this note, we show that the analogous singularities do not arise in the *extended* Weyl–Schrödinger algebra \mathfrak{A} , i.e., for the involutive $*$ -algebra on $L^2(\mathbb{R})$ which is generated by X, P , and $(aX + iI)^{-1}$ for $a \in \mathbb{R}$, again subject to the relation (1.1). Specifically,

Theorem 2.1. *Let $A \in \mathfrak{A}$ be given, and suppose A has positive spectrum, i.e. that $\langle f, Af \rangle \geq 0$, for all $f \in \mathcal{S}$; then A is a finite sum of quadratic terms, H^*H for some finite subset of elements H in \mathfrak{A} .*

Remark 2.2. The example (1.3) shows that the elements H in the expression $A = \Sigma H^*H$ cannot in general be chosen from \mathfrak{A}_0 , even if A is initially given in \mathfrak{A}_0 . The proof of Theorem 2.1 is relatively long, and it consists of three separate ideas each of which may perhaps be of independent interest. For the convenience of the reader, we have therefore broken down the proof in three separate sections to follow.

3. States on \mathfrak{A} and their representations

States on \mathfrak{A} induce representations, and we shall establish extension properties for the representations.

Proof of Theorem 2.1. (Step one.) Suppose that some element A in \mathfrak{A} is *not* a finite sum of the specified type of elements H^*H , for $H \in \mathfrak{A}$. Let the cone $\mathcal{K} \subset \mathfrak{A}$ be spanned (algebraically) by the elements I , and H^*H for $H \in \mathfrak{A}$. Then \mathcal{K} is a convex cone in \mathfrak{A} , and, by assumption, $A \notin \mathcal{K}$. We may then find a linear functional ω on \mathfrak{A} which separates the two, i.e., such that

$$\omega(A) < 0, \quad \text{but} \quad \omega(H^*H) \geq 0 \quad \text{for all } H \in \mathfrak{A}. \quad (3.1)$$

We appeal to (one of the formulations of) the Hahn–Banach theorem for this. Hence we need to know that the (algebraically defined) cone \mathcal{K} is closed in \mathfrak{A} relative to the topology $\sigma(\mathfrak{A}, \mathfrak{A}^*)$ on \mathfrak{A} . Recall, \mathfrak{A}^* denotes the algebraic dual of \mathfrak{A} , i.e. *all* linear functionals on \mathfrak{A} . We may conclude that \mathcal{K} is closed, as specified, from the result of Schmüdgen [Sc1–2]. (This theorem is for the Weyl algebra, but can easily be adapted to the present context.)

Now, let π denote the GNS-representation generated by ω , and let Ω be the corresponding cyclic vector in the representation space $\mathcal{H} = \mathcal{H}_\omega$, cf., formula (2.4) above.

We have the

Lemma 3.1. *The operator $\pi(x)$ with dense domain $\pi(\mathfrak{A})\Omega$ in \mathcal{H} is essentially selfadjoint.*

Proof. Note that $\pi(x)$ is symmetric since the identity $x^* = x$ holds in the Weyl algebra. Then we have the following “quadratic form”–identity valid on the specified dense set of vectors, i.e.,

$$\begin{aligned} \langle \pi(a)\Omega, \pi(x)\pi(b)\Omega \rangle &= \omega(a^*(xb)) = \omega((xa)^*b) \\ &= \langle \pi(x)\pi(a)\Omega, \pi(b)\Omega \rangle. \end{aligned}$$

This shows that $\pi(x)$ is symmetric on its domain. To show that $\pi(x)$ is further essentially selfadjoint, we need to verify that each of the two spaces, $(\pi(x) \pm iI)\pi(\mathfrak{A})\Omega$ is dense in \mathcal{H} . We verify this for $\pi(x) + iI$. The other case is the same, *mutatis mutandis*. If $\psi \in \mathcal{H}$ is given to be in the orthogonal complement, then

$$\langle \psi, (\pi(x) + iI)\pi(b)\Omega \rangle = 0 \quad (3.2)$$

for all $b \in \mathfrak{A}$. Since $(x + i)^{-1} \in \mathfrak{A}$, this holds, in particular, for $(x + i)^{-1}a$ whenever $a \in \mathfrak{A}$. But $(\pi(x) + iI)\pi((x + i)^{-1}a) = \pi(a)$, so we conclude from (3.2), with $b = (x + i)^{-1}a$, that $\langle \psi, \pi(a)\Omega \rangle = 0$. Since Ω is cyclic, it follows that $\psi = 0$ as asserted. This concludes the proof of the lemma.

4. Dilations of representations

Let π be the representation introduced in Sect. 3 above. In this section, we shall study the operator $\pi(p)$. Naturally this operator $\pi(p)$ cannot be expected to be essentially selfadjoint, although it is symmetric. (The element from (1.3) above illustrates this point.)

The following theorem allows us to get around this difficulty. It is a result about selfadjoint *dilations* of Hermitian representations of the Weyl algebra (*not* the extended algebra), and it was first proved, in a special case, in [Jo-Mu], and then, in full generality in [We]. For further details, see also [Jo1–2]. While it is stated in a different form, in the above references, we shall use it in the following equivalent formulation.

Lemma 4.1. ([We]). *Let π be a Hermitian representation of the Weyl algebra W with dense invariant domain \mathcal{D} in a given Hilbert space \mathcal{H} , and suppose $\pi(x)$ is essentially selfadjoint on \mathcal{D} . Then there is a Hermitian representation $\tilde{\pi}$, acting on some Hilbert space $\tilde{\mathcal{H}}$ containing \mathcal{H} , and extending π . Specifically, the domain \mathcal{D} of π is contained in that of $\tilde{\pi}$, and*

$$\tilde{\pi}(a)f = \pi(a)f \tag{4.1}$$

holds for all $a \in W$, and all $f \in \mathcal{D}$. Moreover $\tilde{\pi}(x)^2 + \tilde{\pi}(p)^2$ is essentially selfadjoint on the domain of $\tilde{\pi}$. The subspace \mathcal{H} is reducing for the unitary one-parameter group \tilde{U}_t on $\tilde{\mathcal{H}}$ which is generated by $\tilde{\pi}(x)$, and we have the commutation relation,

$$\tilde{U}_t \tilde{\pi}(p) \tilde{U}_t^* = \tilde{\pi}(p) - t\tilde{I} \tag{4.2}$$

for all $t \in \mathbb{R}$, where \tilde{I} denotes the identity operator on $\tilde{\mathcal{H}}$.

Proof (Sketch). Let U_t be the unitary one-parameter group on \mathcal{H} which is generated by the selfadjoint closure of $\pi(x)$. It is well known [Ak-GI] that the set of selfadjoint dilations $\tilde{\pi}(p)$ of the given symmetric operator $\pi(p)$ is non-empty. Let $(\tilde{\pi}(p), \tilde{\mathcal{H}}_0)$ be such a dilation, see [Ak-GI] and [Jo-Mu] for details; and let $E(d\lambda)$ be the corresponding orthogonal projection valued measure; i.e., $E(\cdot)$ takes values in the orthogonal projections of $\tilde{\mathcal{H}}_0$, and

$$\tilde{\pi}(p) = \int_{-\infty}^{\infty} \lambda E(d\lambda), \tag{4.3}$$

while $\tilde{\pi}(p)$ extends $\pi(p)$ on the dense domain \mathcal{D} in $\mathcal{H} \subset \tilde{\mathcal{H}}_0$. Let Q_0 be the orthogonal projection of $\tilde{\mathcal{H}}_0$ onto the subspace \mathcal{H} , and let $F(\cdot) = Q_0 E(\cdot) Q_0$. Then we seek $F(\cdot)$ of this form such that

$$U_t F(d\lambda) U_t^* = F(d\lambda + t) \tag{4.4}$$

(which is the compression to \mathcal{H} of a relation which is equivalent to (4.2) above.) Let α_t denote the automorphic action of \mathbb{R} by translation on the set of all “quasi” spectral resolutions $F(\cdot)$ associated to $\pi(p)$. Then (4.4) may be written in the form

$$U_t \alpha_{-t}(F) U_t^* = F; \tag{4.5}$$

and a resolution F , of the desired form, may be found by reference to the fixed point theorem of Markoff–Kakutani [D-S], or by use of the amenability of \mathbb{R} . Once

a solution F to (4.4) is found, then the action of \tilde{U}_t on the corresponding dilation space $\tilde{\mathcal{H}}$ is dictated by the commutation relation. We may take $\tilde{\mathcal{H}}$ to be generated by the space \mathcal{H} , and the associated representation of the extended Weyl algebra \tilde{W} on $\tilde{\mathcal{H}}$. For more details, see [Jo-Mu] and [We]. The properties of the chosen compression $F = Q\tilde{E}Q$ are described below:

We have the unitary one-parameter group $U_t, t \in \mathbb{R}$, acting on \mathcal{H} . Once a positive operator valued measure $F(\cdot)$ has been found satisfying the commutation relation (4.4), then an application of the dilation theorem [Jo2, Chapter 4] provides us with an operator system $\tilde{U}_t, \tilde{E}(\cdot)$, acting in a bigger Hilbert space and satisfying relation

$$\tilde{U}_t \tilde{E}(d\lambda) \tilde{U}_t^* = \tilde{E}(d\lambda + t), \quad t \in \mathbb{R} . \tag{4.4}$$

The original Hilbert space \mathcal{H} reduces the unitary group \tilde{U}_t , and the restriction to \mathcal{H} coincides with U_t . If Q denotes the projection onto \mathcal{H} , then $F(\cdot) = Q\tilde{E}(\cdot)Q$, and $\tilde{E}(\cdot)$ is an orthogonal projection valued measure.

If $V_s, s \in \mathbb{R}$, denotes the unitary one-parameter group on $\tilde{\mathcal{H}}$ which is generated by $\tilde{\pi}(p)$, then we have the Weyl form of the commutation relation, i.e.,

$$\tilde{U}_t V_s = e^{-ist} V_s \tilde{U}_t, \quad s, t \in \mathbb{R} . \tag{4.6}$$

In fact, (4.6) follows directly from (4.2) above by use of general commutation theory, see e.g., [Jo-Mo, Chapter 6].

Formula (4.6), and Nelson's theorem [Ne], now imply that the quadratic operator, $\tilde{\pi}(x)^2 + \tilde{\pi}(p)^2$ is essentially selfadjoint as in the statement of the lemma. This concludes the proof.

5. The Stone-von Neumann theorem

Having the exponentiated commutation relation (4.6), we may now appeal to the Stone-von Neumann uniqueness theorem. (For a version of this theorem which does not assume separability of $\tilde{\mathcal{H}}$, the reader is referred to [Or] and [Jo2, Chapter 4].) Up to unitary equivalence, the system (\tilde{U}, V) on $\tilde{\mathcal{H}}$ must necessarily be the direct sum of identical copies of the Schrödinger representation σ , from Sect. 1 above, but now in integrated form. To state the Stone-von Neumann theorem, let \mathcal{M} be a Hilbert space, and let $L^2(\mathbb{R}, \mathcal{M})$ be the corresponding L^2 -space of \mathcal{M} -valued functions defined on the real line. The uniqueness theorem then yields the existence of some \mathcal{M} , and a unitary operator, $W: \tilde{\mathcal{H}} \rightarrow L^2(\mathbb{R}, \mathcal{M})$, such that

$$(W\tilde{U}_t W^*)f(x) = f(x + t), \tag{5.1}$$

$$(WV_s W^*)f(x) = e^{isx} f(x) \tag{5.2}$$

where $f \in L^2(\mathbb{R}, \mathcal{M})$, and $t, s, x \in \mathbb{R}$.

We now return to the proof of Theorem 2.1. Recall that a state ω was chosen such that $\omega(A) < 0$, and yet $\omega \geq 0$ on a certain cone.

For the state ω (which was used to separate the given element A from the “quadratic” cone \mathcal{K}) we have, cf., (2.4) above,

$$\begin{aligned} \omega(A) &= \langle \Omega, \pi(A)\Omega \rangle \\ &= \langle \Omega, \tilde{\pi}(A)\Omega \rangle \\ &= \langle W\Omega, W\tilde{\pi}(A)W^*W\Omega \rangle \\ &= \langle W\Omega, \sigma_{\mathcal{M}}(A)W\Omega \rangle \end{aligned} \tag{5.3}$$

where $\sigma_{\mathcal{M}}(\cdot)$ denotes the Schrödinger representation acting on \mathcal{M} -vector valued functions. The vacuum vector $f_0 := W\Omega \in L^2(\mathbb{R}, \mathcal{M})$ is a C^∞ -vector for this representation. By a result in [Pou, Sect. 5], this means that, each function

$$x \mapsto \langle m, f_0(x) \rangle_{\mathcal{M}} \quad \text{on } \mathbb{R}, \tag{5.4}$$

for fixed $m \in \mathcal{M}$, is in the (scalar valued) Schwartz space of \mathbb{R} . The action of the operator $\sigma_{\mathcal{M}}(A)$ on f_0 is just the given operator action of A in the x -variable. With this convention, and notation, formula (5.3) may therefore be rewritten in the form

$$\omega(A) = \int_{-\infty}^{\infty} \langle f_0(x), (Af_0)(x) \rangle_{\mathcal{M}} dx \tag{5.5}$$

where the integral is convergent due to the stated Schwartz-type property of f_0 , and where $\langle \cdot, \cdot \rangle_{\mathcal{M}}$ denotes the Hilbert space-inner product in \mathcal{M} . If an orthonormal basis is introduced in \mathcal{M} , we may break down the right hand side as a sum (over the index set of the chosen basis) of terms of the same form (5.5), but now with scalar valued functions, i.e., a family of scalar valued functions (5.4) where the constant vector m runs over the chosen orthonormal basis in \mathcal{M} . But each term in the resulting sum, on the right hand side of (5.5), satisfies $\int \langle \cdot, \cdot \rangle dx \geq 0$ if A is assumed to be of positive spectral type. It follows that $\omega(A) \geq 0$ which contradicts the initial estimate, stated in (3.1) above. This concludes the proof of Theorem 2.1.

6. Concluding remarks

It follows from the Theorem (2.1) that the element $T = (N - I)(N - 2I)$ from Sect. 1 may be expressed in the form $T = \sum_i H_i^* H_i$ for some finite set of elements in the extended Weyl algebra \mathfrak{A} . We note that a direct computation reveals that it is possible to do this with just a single term in the sum. In fact, if

$$C = \frac{1}{2} \left(\frac{d^2}{dx^2} + \alpha(x) \frac{d}{dx} + \beta(x) \right) \tag{6.1}$$

or equivalently

$$C = \frac{1}{2} (-P^2 + \alpha(x) i P + \beta(x))$$

then we get

$$T = C^* C \tag{6.2}$$

with the following choice for the two rational functions $\alpha(x)$ and $\beta(x)$ in (6.1):

$$\alpha(x) = \frac{4x^3 - 2x}{2x^2 + 1} \quad \text{and} \quad \beta(x) = \frac{2x^4 - x^2 + 5}{2x^2 + 1}.$$

If conversely

$$T = \sum_i H_i^* H_i \quad (\text{finite sum with } H_i \in \mathfrak{A}), \quad (6.3)$$

then it follows from elementary facts on second order differential operators that the elements H_i must be of the form, $H_i = f_i(x)C$, where again the operator C is given by (6.1), and where $f_i(x)$ is viewed as a multiplication operator. By comparing highest order terms in (6.3), we conclude that $\sum_i |f_i(x)|^2 = 1$. But then

$$\begin{aligned} T &= \sum_i H_i^* H_i = \sum_i \overline{C^* f_i(x)} f_i(x) C \\ &= C^* \left(\sum_i \overline{f_i(x)} f_i(x) \right) C = C^* C. \end{aligned}$$

This displays the possible non-uniqueness for the representation (6.3). The amount of ambiguity is labeled by partitions of unity as specified.

We finally note that the explicit formulae for the two coefficient functions $\alpha(x)$ and $\beta(x)$ of the second order differential operator C may be found by using the following two facts: First we have, $T(A^{*n}f_0) = (n-1)(n-2)A^{*n}f_0$ holding for all $n = 0, 1, 2, \dots$ where A^* denotes the creation operator. It follows that each term H_i in (6.3) must satisfy, $H_i(A^{*n}f_0) = 0$, $n = 1, 2$. Each H_i must therefore be of second order, and have a representation as specified.

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* The theorem which is referred to in the *Summary* above is from [Po], but the result from [Po] is in fact a version of an extension theorem which was proved first by Arveson in the context of bounded operators; W.B. Arveson, “Subalgebras of C^* -algebras,” *Acta Math.* **123**, 141–244 (1969)