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Stephen Bruce Sontz
Centro de Investigación en Matemáticas, A.C. (CIMAT) Guanajuato, Gto. 36023, Mexico, sontz@cimat.mx

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PAULI MATRICES: A TRIPLE OF ACCARDI COMPLEMENTARY OBSERVABLES

STEPHEN BRUCE SONTZ*

Dedicated to Professor Leonard Gross on the occasion of his 88th birthday

Abstract. The definition due to Accardi of a pair of complementary observables is adapted to the context of the Lie algebra $su(2)$. We show that the pair of Pauli matrices A, B associated to the unit directions α and β in $\mathbb{R}^3$ are Accardi complementary if and only if α and β are orthogonal if and only if A and B are orthogonal. In particular, any pair of the standard triple of Pauli matrices is complementary.

1. Introduction

The idea of complementarity has hung around quantum theory from its earliest days as explained in [4]. But the exact encoding of that idea as a rigorous, mathematical definition has been elusive. A rather interesting definition of complementary pairs originates in 1984 in Accardi's paper [1], which is more fully presented in [3]. Well before that an example of complementarity for an explicit pair of observables was given by Schwinger in [5] in 1960. These definitions of complementarity are extended in this note from pairs of observables to any set, finite or infinite, of observables. Also the recent paper [2] of Accardi and Lu has an alternative definition of complementary sets of observables given in terms of a more general definition of complementarity of sub-$*$-algebras of a $*$-algebra. See Definition 5 in [2] for the details.

2. Preliminaries

In this section we review some standard material in order to establish notation and context. We use the standard notation for the Pauli matrices:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

For any vector $\alpha = (\alpha_1, \alpha_2, \alpha_3) \in \mathbb{R}^3$ we let

$$\alpha \cdot \sigma := \alpha_1\sigma_1 + \alpha_2\sigma_2 + \alpha_3\sigma_3 = \begin{pmatrix} \alpha_3 & \alpha_1 - i\alpha_2 \\ \alpha_1 + i\alpha_2 & -\alpha_3 \end{pmatrix}.$$

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* Corresponding author.

We denote the unit sphere in $\mathbb{R}^3$ as

$$S^2 := \{\alpha = (\alpha_1, \alpha_2, \alpha_3) \in \mathbb{R}^3 \mid ||\alpha||^2 := \alpha_1^2 + \alpha_2^2 + \alpha_3^2 = 1\}.$$

For a 2×2 matrix A we will use the normalized trace, $\operatorname{tr} A := (a+d)/2$, where

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \qquad \text{for } a, b, c, d \in \mathbb{C}.$$

Since $\sigma_1^2 = \sigma_2^2 = \sigma_3^2 = I$, where I is the 2×2 identity matrix, we have that $\operatorname{tr} \sigma_1^2 = \operatorname{tr} \sigma_2^2 = \operatorname{tr} \sigma_3^2 = 1$. Also, $\operatorname{tr} \sigma_1 = \operatorname{tr} \sigma_2 = \operatorname{tr} \sigma_3 = 0$. We denote the set of hermitian (i.e., self-adjoint), traceless 2×2 matrices with complex entries by

$$su(2) := \{A \mid A = A^*, \operatorname{tr} A = 0\}.$$

Here M^* denotes the adjoint (complex conjugate, transposed) of M, where M is any matrix, even a rectangular one. Then $su(2)$ is the Lie algebra of the Lie group $SU(2)$. It is a vector space over the reals $\mathbb{R}$, and the map $\Sigma : \mathbb{R}^3 \to su(2)$ given for each $\alpha \in \mathbb{R}^3$ by $\Sigma(\alpha) := \alpha \cdot \sigma$ is a linear, onto isomorphism of real vector spaces. In particular, for all $\alpha \in \mathbb{R}^3$ we have $(\alpha \cdot \sigma)^* = \alpha \cdot \sigma$ and

$$\operatorname{tr}(\alpha \cdot \sigma) = 0. \tag{2.1}$$

Moreover, we give $\mathbb{R}^3$ the standard inner product, denoted $\langle \cdot, \cdot \rangle$, and we give $su(2)$ the inner product, also with the same notation, by restricting to $su(2)$ the normalized Hilbert-Schmidt inner product:

$$\langle A, B \rangle := \operatorname{tr}(A^* B) \quad \text{for all } 2 \times 2 \text{ matrices } A, B.$$

Then Σ is a unitary isomorphism of $\mathbb{R}^3$ onto $su(2)$. Explicitly, this says that

$$\langle \Sigma(\alpha), \Sigma(\beta) \rangle = \langle \alpha \cdot \sigma, \beta \cdot \sigma \rangle = \operatorname{tr}\big((\alpha \cdot \sigma)(\beta \cdot \sigma)\big) = \langle \alpha, \beta \rangle \quad \text{for all } \alpha, \beta \in \mathrm{R}^3. \tag{2.2}$$

Also, $\{\sigma_1, \sigma_2, \sigma_3\}$ is an orthonormal basis of $su(2)$. The matrices in $su(2)$, which are all self-adjoint, act on the Hilbert space $\mathbb{C}^2$ with its standard inner product and, as such, represent quantum physical observables.

Using this notation and standard properties of the Pauli matrices, we have $(\alpha \cdot \sigma)^2 = ||\alpha||^2 I$. From this one immediately has that the spectrum of $\alpha \cdot \sigma$ is $\operatorname{Spec}(\alpha \cdot \sigma) = \{ -||\alpha||^2, ||\alpha||^2 \}$. This motivates calling $\alpha \cdot \sigma$ for $\alpha \in S^2$ the *Pauli matrix in the direction* α. Also, in quantum physics $(\hbar/2)(\alpha \cdot \sigma)$ is called the *spin matrix in the direction* α, where $\hbar > 0$ is the normalized Planck constant. The results of this paper are given in terms of the Pauli matrices $\alpha \cdot \sigma$ for $\alpha \in S^2$. However, they are easily modified to apply to the spin matrices.

3. Results

Theorem 3.1. (Accardi in [1]) *Suppose Q and P are the standard self-adjoint realizations of the position and momentum operators acting in the Hilbert space $L^2(\mathbb{R})$. Let S_1, S_2 be bounded Borel subsets of $\mathbb{R}$. Then $E_Q(S_1)E_P(S_2)$ is a trace class operator, where E_Q (resp., E_P) is the projection valued measure on $\mathbb{R}$ associated by the spectral theorem with the self-adjoint operator Q (resp., P). Moreover,*

$$Tr\big(E_Q(S_1)E_P(S_2)\big) = \mu_L(S_1)\mu_L(S_2),$$

where Tr denotes the trace of a trace class operator and μ_L is the rescaling of Lebesgue measure μ of $\mathbb{R}$ given by $\mu_L = (2\pi)^{-1/2}\,\mu$.

We use this theorem to motivate a definition in the context of this paper.

Definition 3.2. Let $A, B \in su(2)$ lie on the unit sphere, i.e., $\operatorname{tr} A^2 = \operatorname{tr} B^2 = 1$, with E_A, E_B being their projection valued measures. Then we say that A, B are *Accardi complementary* if for all Borel subsets S_1, S_2 of $\mathbb{R}$ we have that

$$\big\langle E_A(S_1), E_B(S_2)\big\rangle = \operatorname{tr}\big(E_A(S_1)E_B(S_2)\big) = \mu_B(S_1)\mu_B(S_2), \tag{3.1}$$

where μ_B is the symmetric Bernoulli probability measure on $\mathbf{R}$ supported on the set $\operatorname{Spec} A = \operatorname{Spec} B = \{-1, +1\}$, that is $\mu_B(\{-1\}) = \mu_B(\{+1\}) = 1/2$.

This definition follows the original motivation of this concept in [1] where it is shown that (3.1) is equivalent to saying that measuring a value of A gives no further information on what the value of B will be on a subsequent measurement of it, and *vice versa*.

We now want to find the projection valued measure for any $A \in su(2)$ with norm 1. To do this we first use the isomorphism Σ to write $A = \alpha \cdot \sigma$ for a unique $\alpha \in S^2$ in order to find its eigenvectors.

Proposition 3.3. *Suppose that $\alpha \in S^2$. Then a normalized eigenvector of the matrix $\alpha \cdot \sigma$ with eigenvalue $+1$ is the column vector*

$$\psi_\alpha^+ := \frac{1}{2^{1/2}(1+\alpha_3)^{1/2}} \begin{pmatrix} 1+\alpha_3 \\ \alpha_1 + i\alpha_2 \end{pmatrix} \in \mathbb{C}^2 \quad \text{if } \alpha_3 \neq -1. \tag{3.2}$$

And a normalized eigenvector of the matrix $\alpha \cdot \sigma$ with eigenvalue -1 is the column vector

$$\psi_\alpha^- := \frac{1}{2^{1/2}(1-\alpha_3)^{1/2}} \begin{pmatrix} -1+\alpha_3 \\ \alpha_1 + i\alpha_2 \end{pmatrix} \in \mathbb{C}^2 \quad \text{if } \alpha_3 \neq +1. \tag{3.3}$$

Proof. The eigenvalue equations (with unknowns x, y) are

$$\begin{pmatrix} \alpha_3 & \alpha_1 - i\alpha_2 \\ \alpha_1 + i\alpha_2 & -\alpha_3 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \pm \begin{pmatrix} x \\ y \end{pmatrix}, \tag{3.4}$$

where the sign $+$ (resp., $-$) corresponds to eigenvalue $+1$ (resp., -1). Using the hypothesis $||\alpha||^2 = 1$, one easily checks that the vectors in (3.2) and (3.3) satisfy (3.4) with the appropriate sign and that they have norm 1. □

Now we find the projection valued measure $E_{\alpha\cdot\sigma}$ of $\alpha \cdot \sigma$ for $\alpha \in S^2$.

Theorem 3.4. *Suppose that $\alpha \in S^2$. Then for the two non-trivial subsets of* $\operatorname{Spec}(\alpha \cdot \sigma) = \{-1, +1\}$ *we have that*

$$E_{\alpha\cdot\sigma}(\{+1\}) = \frac{1}{2} \begin{pmatrix} 1+\alpha_3 & \alpha_1 - i\alpha_2 \\ \alpha_1 + i\alpha_2 & 1-\alpha_3 \end{pmatrix} = \frac{1}{2}(I + \alpha\cdot\sigma) \tag{3.5}$$

and

$$E_{\alpha\cdot\sigma}(\{-1\}) = \frac{1}{2} \begin{pmatrix} 1-\alpha_3 & -\alpha_1 + i\alpha_2 \\ -\alpha_1 - i\alpha_2 & 1+\alpha_3 \end{pmatrix} = \frac{1}{2}(I - \alpha\cdot\sigma) \tag{3.6}$$

Proof. Using Dirac notation, we have $E_{\alpha\cdot\sigma}(\{+1\}) = |\psi_\alpha^+\rangle\langle\psi_\alpha^+|$, where ψ_α^+ is given in (3.2). Then one can calculate the matrix in the middle of (3.5) directly from this formula by multiplying the column matrix $|\psi_\alpha^+\rangle$ by the row matrix $\langle\psi_\alpha^+| = |\psi_\alpha^+\rangle^*$. Or one can verify that the expression on the rightmost side of (3.5) is a projection whose range is spanned by ψ_α^+.

But the most elegant proof is to note that $E_{\alpha\cdot\sigma}(\{+1\}) = \chi_1(\alpha\cdot\sigma)$ by spectral theory, where χ_1 is the characteristic function of the set $\{1\}$, and then to use interpolation with Lagrange polynomials which says every function f of a 2×2 matrix A is equal to a polynomial p of degree at most 1 of A, where p must satisfy $p = f$ on the spectrum of A. Therefore we have $\chi_1(x) = ax + b$ for all $x \in \mathrm{Spec}\,(\alpha\cdot\sigma) = \{-1,+1\}$ for unknown coefficients a, b. This gives the equations

$$1 = \chi_1(1) = a + b \quad \text{and} \quad 0 = \chi_1(-1) = a - b,$$

whose solution clearly is $a = b = 1/2$. Thus, $\chi_1(x) = (1/2)(1+x) =: p_1(x)$ for all $x \in \{-1,+1\}$. Finally, $E_{\alpha\cdot\sigma}(\{+1\}) = \chi_1(\alpha\cdot\sigma) = p_1(\alpha\cdot\sigma) = \frac{1}{2}(I + \alpha\cdot\sigma)$.

The expressions in (3.6) can be proved similarly or, even quicker, by using that $E_{\alpha\cdot\sigma}(\{-1\}) = I - E_{\alpha\cdot\sigma}(\{+1\})$. □

Of course, $E_{\alpha\cdot\sigma}(\{-1,+1\}) = I$ and $E_{\alpha\cdot\sigma}(\{\emptyset\}) = 0$ by spectral theory, where $\emptyset$ denotes the empty set and 0 denotes the zero operator.

Also, the expressions in (3.5) and (3.6) seem to indicate that the singularities in (3.2) and (3.3) are removable. But that is not true as can be seen by writing those expressions in spherical coordinates.

Theorem 3.5. *For each subset $S \subset \{-1,+1\}$, we have $\mathrm{tr}\, E_{\alpha\cdot\sigma}(S) = \mu_B(S)$ for all $\alpha \in S^2$. In short, $\mathrm{tr} \circ E_{\alpha\cdot\sigma} = \mu_B$ for all $\alpha \in S^2$.*

Proof. There are four such subsets S. So we prove this in each of those four cases. For $S = \emptyset$ the result is trivial. For $S = \{-1,+1\}$ we have

$$\mathrm{tr}\, E_{\alpha\cdot\sigma}(S) = \mathrm{tr}\, E_{\alpha\cdot\sigma}(\{-1,+1\}) = \mathrm{tr}\, I = 1 = \mu_B(\{-1,+1\}) = \mu_B(S).$$

Finally, we obtain immediately from (3.5) and (3.6) that $\mathrm{tr}\, E_{\alpha\cdot\sigma}(\{+1\}) = \mathrm{tr}\, E_{\alpha\cdot\sigma}(\{-1\}) = 1/2$ for all $\alpha \in S^2$. Since $\mu_B(\{+1\}) = \mu_B(\{-1\}) = 1/2$, we have proved the remaining two cases as well. □

This basic theorem shows how spectral theory and the state tr give rise to the probability measure μ_B. We now are ready for the main result of this paper.

Theorem 3.6. *Suppose $\alpha, \beta \in S^2$. Then $\alpha\cdot\sigma$, $\beta\cdot\sigma$ is Accardi complementary if and only if $\langle \alpha\cdot\sigma, \beta\cdot\sigma\rangle = \langle \alpha, \beta\rangle = 0$, where the first inner product is that of $su(2)$ and the second is the standard inner product on $\mathbb{R}^3$.*

Proof. It suffices to compute $\mathrm{tr}\big(E_{\alpha\cdot\sigma}(S_1)E_{\beta\cdot\sigma}(S_2)\big)$ for all the subsets S_1, S_2 of $\{-1,+1\}$. If $S_1 = \emptyset$, then

$$\mathrm{tr}\big(E_{\alpha\cdot\sigma}(S_1)E_{\beta\cdot\sigma}(S_2)\big) = \mathrm{tr}(0\, E_{\beta\cdot\sigma}(S_2)) = \mathrm{tr}(0) = 0$$

while

$$\mu_B(S_1)\mu_B(S_2) = 0 \cdot \mu_B(S_2) = 0.$$

This shows that (3.1) holds for this case. The case $S_2 = \emptyset$ is proved similarly. If $S_1 = \{-1,+1\}$, then

$$\mathrm{tr}\big(E_{\alpha\cdot\sigma}(S_1)E_{\beta\cdot\sigma}(S_2)\big) = \mathrm{tr}(I\, E_{\beta\cdot\sigma}(S_2)) = \mathrm{tr}(E_{\beta\cdot\sigma}(S_2))$$

while

$$\mu_B(S_1)\mu_B(S_2) = 1 \cdot \mu_B(S_2) = \mu_B(S_2).$$

So (3.1) holds in this case by Theorem 3.5. The case $S_2 = \{-1, +1\}$ is proved similarly.

We now consider the cases when both S_1 and S_2 contain exactly one element. In all of these remaining cases we have that $\mu_B(S_1)\,\mu_B(S_2) = (1/2)(1/2) = 1/4$.

For the case $S_1 = S_2 = \{+1\}$, we have

$$\begin{aligned}
&\operatorname{tr}\big(E_{\alpha\cdot\sigma}(S_1)E_{\beta\cdot\sigma}(S_2)\big) = \operatorname{tr}\big(E_{\alpha\cdot\sigma}(\{+1\})E_{\beta\cdot\sigma}(\{+1\})\big) \\
&= \frac{1}{4}\operatorname{tr}\big((I + \alpha\cdot\sigma)(I + \beta\cdot\sigma)\big) = \frac{1}{4}\operatorname{tr}\big(I + \alpha\cdot\sigma + \beta\cdot\sigma + (\alpha\cdot\sigma)(\beta\cdot\sigma)\big) \\
&= \frac{1}{4}(1 + 0 + 0 + \langle\alpha, \beta\rangle) = \frac{1}{4}(1 + \langle\alpha, \beta\rangle).
\end{aligned}$$

Here in the fourth equality we used (2.1) and (2.2). Therefore, (3.1) holds in this case if and only if $\langle\alpha, \beta\rangle = 0$.

For the case $S_1 = S_2 = \{-1\}$, we have

$$\begin{aligned}
&\operatorname{tr}\big(E_{\alpha\cdot\sigma}(S_1)E_{\beta\cdot\sigma}(S_2)\big) = \operatorname{tr}\big(E_{\alpha\cdot\sigma}(\{-1\})E_{\beta\cdot\sigma}(\{-1\})\big) \\
&= \frac{1}{4}\operatorname{tr}\big((I - \alpha\cdot\sigma)(I - \beta\cdot\sigma)\big) = \frac{1}{4}\operatorname{tr}\big(I - \alpha\cdot\sigma - \beta\cdot\sigma + (\alpha\cdot\sigma)(\beta\cdot\sigma)\big) \\
&= \frac{1}{4}(1 + \langle\alpha, \beta\rangle).
\end{aligned}$$

So (3.1) holds in this case if and only if $\langle\alpha, \beta\rangle = 0$.

Next we consider the case $S_1 = \{+1\}$ and $S_2 = \{-1\}$. Then we have

$$\begin{aligned}
&\operatorname{tr}\big(E_{\alpha\cdot\sigma}(S_1)E_{\beta\cdot\sigma}(S_2)\big) = \operatorname{tr}\big(E_{\alpha\cdot\sigma}(\{+1\})E_{\beta\cdot\sigma}(\{-1\})\big) \\
&= \frac{1}{4}\operatorname{tr}\big((I + \alpha\cdot\sigma)(I - \beta\cdot\sigma)\big) = \frac{1}{4}\operatorname{tr}\big(I + \alpha\cdot\sigma - \beta\cdot\sigma - (\alpha\cdot\sigma)(\beta\cdot\sigma)\big) \\
&= \frac{1}{4}(1 - \langle\alpha, \beta\rangle).
\end{aligned}$$

Again (3.1) holds in this case if and only if $\langle\alpha, \beta\rangle = 0$.

The remaining case $S_1 = \{-1\}$ and $S_2 = \{+1\}$ is proved similarly to the previous case. □

Definition 3.7. A subset of the unit sphere in $su(2)$ is *Accardi complementary* if every subset of it with exactly 2 elements is Accardi complementary.

Corollary 3.8. *Let α, β, γ be an orthonormal basis of $\mathbb{R}^3$. Then any pair of matrices in the set $\{\alpha\cdot\sigma, \beta\cdot\sigma, \gamma\cdot\sigma\}$ is Accardi complementary. In particular the triple of Pauli matrices $\{\sigma_1, \sigma_2, \sigma_3\}$ is Accardi complementary.*

This result encodes the common knowledge in quantum physics which says that measuring the spin of a spin 1/2 particle in some direction gives no information about subsequent spin measurements in any orthogonal direction. See [1] for more on this point.

Corollary 3.9. *Every subset of the unit sphere in $su(2)$ with 4 or more elements is not Accardi complementary.*

As an anonymous referee has kindly pointed out, these results express in the language of Accardi complementarity the known fact that the maximum number of mutually unbiased bases in $\mathbb{C}^2$ is 3.

4. Concluding Remarks

There are properties of sets in mathematics which are of *finite type*, that is, a set has the property if and only if every finite subset of it has the property. The property of linear independence for subsets of a vector space is a property of finite type.

There are other properties of sets which are of *unary type*, that is, a set has the property if and only if every subset with exactly 1 element has the property. The property of a set of vectors in a normed vector being normalized is a property of unary type.

There are other properties of sets which are of *binary type*, that is, a set has the property if and only if every subset with exactly 2 elements has the property. The property that a set of vectors in a Hilbert space is orthogonal is a property of binary type. We have shown that Accardi complementarity is a meaningful property of binary type by giving examples of triples each of whose pairs is Accardi complementary.

Next, let us note that the main theorem of this paper indicates that the *symmetric* Bernoulli probability measure μ_B is in some sense a natural measure on $\mathrm{Spec}\,(\alpha \cdot \sigma)$ for any $\alpha \in S^2$. Of course, μ_B is the unique probability measure on $\mathrm{Spec}\,(\alpha \cdot \sigma) = \{-1, +1\}$ with maximum entropy or, equivalently, with minimal information. This is its relevant property for this topic. Of course, μ_B is also the normalized Haar measure on the finite multiplicative group $\{-1, +1\}$.

Theorem 3.6 clearly should generalize to any irreducible representation of $su(2)$, that is to say in terms of quantum physics, to any particle with spin $n\hbar/2$ with $n \geq 0$ being an integer.

Finally, after the preliminary version of this paper was finished, I learned about the results in [2], where a stronger notion of complementarity is introduced for arbitrary sets of observables and examples of these are given and studied.

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Stephen Bruce Sontz: Centro de Investigación en Matemáticas, A.C. (CIMAT)
Guanajuato, Gto. 36023, Mexico
E-mail address: sontz@cimat.mx
URL: http://cimat.mx