Analysis of 1 and 2 Particle Quantum Systems using Geometric Algebra

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Abstract

When two or more subsystems of a quantum system interact with each other they can become entangled. In this case the individual subsystems can no longer be described as pure quantum states. For systems with only 2 subsystems this entanglement can be described using the Schmidt decomposition. This selects a preferred orthonormal basis for expressing the wavefunction and gives a measure of the degree of entanglement present in the system. The extension of this to the more general case of n subsystems is not yet known. We present a review of this process using the standard representation and apply this method to the geometric algebra representation. This latter form has the advantage of suggesting a generalisation to n subsystems.

1 Introduction

Quantum entanglement in 2-particle systems is currently well understood (for a useful review, including an extensive list of references, see [1]). But the quantum behaviour of many-particle systems is more complicated and less well understood, and it is these systems that are of interest experimentally. The main limitation to the theoretical understanding of such systems is that the techniques which have been developed to analyse 2-particle systems do not easily generalise. Geometric algebra has the advantage that the number of particles being analysed dictates the size of the space but otherwise does not alter the analysis used. In this way, results developed in simple cases (such as the 2-particle system) can be more easily generalised to the n-particle case.

In this paper we focus on 2-state quantum systems in the cases of one and two particles. We start by reviewing the standard matrix-based approach to single and two-particle pure states. We describe the *Schmidt Decomposition*, which provides a measure of the degree of entanglement present in a given system. We then introduce the density matrix to describe both pure and mixed states in a unified manner. We next turn to an analysis of the same systems using the multiparticle spacetime algebra framework developed by Doran, Lasenby and Gull [2, 3, 4]. As a simple application we review the properties of the spin singlet state, frequently encountered in discussions of the Bell inequalities and EPR-type experiments [5].

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2 Single-Particle Pure States

If there is only one particle present in the system then the spinor, $|\psi\rangle \in \mathcal{H}$, can always be written in the form

$$|\psi\rangle = c_0|0\rangle + c_1|1\rangle \tag{1}$$

where $|0\rangle$ and $|1\rangle$ are some pair of orthogonal basis states and c_0 and c_1 are complex coefficients. Alternatively, all information about the state of the particle can be expressed in a polarisation (or spin) vector, $\boldsymbol{P}$, whose components are given by

$$P_i = \langle\hat{\sigma}_i\rangle = \langle\psi|\hat{\sigma}_i|\psi\rangle/\langle\psi|\psi\rangle \tag{2}$$

where the $\hat{\sigma}_i$ are the Pauli matrices

$$\hat{\sigma}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{\sigma}_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \hat{\sigma}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{3}$$

It follows from this definition that $|\boldsymbol{P}| = 1$. In this way the spin state of the particle can be expressed graphically as a point on the 2-sphere, and any evolution of the state of the particle can be thought of as a rotation of the polarisation vector. In many applications this sphere is known as the *Bloch sphere*.

3 2-Particle Systems

Suppose that two particles are described by states belonging to individual Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$. The joint Hilbert space for the interacting system is $\mathcal{H}_1 \otimes \mathcal{H}_2$, consisting of complex superpositions of tensor products of states in the individual spaces. A basis for $\mathcal{H}_1 \otimes \mathcal{H}_2$ is constructed by taking the tensor products of the basis vectors for $\mathcal{H}_1$ and $\mathcal{H}_2$. Therefore any pure state of the composite system, $|\psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$, can be expressed as

$$|\psi\rangle = \sum_{i,j=0,1} c_{i,j}|i\rangle \otimes |j\rangle \equiv \sum_{i,j=0,1} c_{i,j}|i,j\rangle. \tag{4}$$

If more than one of the $c_{i,j}$'s are non-zero then each subsystem is no longer in a pure state and the system is entangled. In order to quantify the degree of entanglement we re-express equation (4) in the form

$$|\psi\rangle = \cos(\alpha/2)|0',0'\rangle + \sin(\alpha/2)|1',1'\rangle, \tag{5}$$

which can always be done via a suitable change of basis. Here, $|0'\rangle$ and $|1'\rangle$ are orthonormal vectors in $\mathcal{H}_1$ and $\mathcal{H}_2$ and $0 \leq \alpha \leq \pi/2$ (so that $\cos(\alpha/2) > \sin(\alpha/2)$). Then $|0',0'\rangle$ can be thought of as the separable state 'closest' to $|\psi\rangle$ and α as the degree of entanglement present in the system. The procedure by which this basis is constructed is the *Schmidt Decomposition*, which we now describe.

3.1 Schmidt Decomposition

An arbitrary wavefunction $|\psi\rangle$ can be rewritten as a sum of two state vectors through a transformation of the basis vectors in the following way [6]. Let $|u\rangle$ and $|v\rangle$ be unit vectors of the first and second particles respectively. Define M by

$$M = \langle u, v|\psi\rangle. \tag{6}$$

$|M|^2$ is nonnegative and bounded so it attains its maximum, $|M_1|^2$, for some $|u_1\rangle$ and $|v_1\rangle$. The choice of $|u_1\rangle$ and $|v_1\rangle$ is not unique since they can at most be determined only up to phase and it is possible that there are other degeneracies as well.

Let $|u'\rangle$ be any state of the first particle which is orthogonal to $|u_1\rangle$, and let ϵ be an arbitrarily small number. Then

$$\left|\,|u_1\rangle + \epsilon|u'\rangle\right|^2 = 1 + \mathcal{O}(\epsilon^2) \tag{7}$$

so that up to order ϵ^2, $|u_1\rangle + \epsilon|u'\rangle$ is a unit vector. We then find that

$$\langle u_1 + \epsilon u', v_1|\psi\rangle = M_1 + \epsilon\langle u', v_1|\psi\rangle \tag{8}$$

so

$$|\langle u_1 + \epsilon u', v_1|\psi\rangle|^2 = |M_1|^2 + 2\mathrm{Re}(\overline{M_1}\epsilon\langle u', v_1|\psi\rangle) + \mathcal{O}(\epsilon^2). \tag{9}$$

But $|u_1\rangle$ was chosen so that the scalar product in Eq. (6) is a maximum. Therefore we must have that

$$\begin{aligned} &|M_1|^2 + 2\mathrm{Re}(\overline{M_1}\epsilon\langle u', v_1|\psi\rangle) \leq |M_1|^2, \\ \implies \quad &\mathrm{Re}(\overline{M_1}\epsilon\langle u', v_1|\psi\rangle) \leq 0. \end{aligned} \tag{10}$$

The choice of phase of $|v_1\rangle$ is arbitrary, however, so to ensure that Eq. (10) is satisfied we must have that

$$\langle u', v_1|\psi\rangle = 0, \qquad \forall \quad u' \in \mathcal{H}_1^{u_1^\perp} = \{u' \in \mathcal{H}_1 | \langle u_1|u'\rangle = 0\}. \tag{11}$$

Similarly, we can show that the same restriction applies to the second particle so that

$$\langle u_1, v'|\psi\rangle = 0, \qquad \forall \quad v' \in \mathcal{H}_2^{v_1^\perp} = \{v' \in \mathcal{H}_2 | \langle v_1|v'\rangle = 0\}. \tag{12}$$

If we now define a new wavefunction

$$|\psi'\rangle = |\psi\rangle - M_1|u_1, v_1\rangle \tag{13}$$

then $|\psi'\rangle$ also satisfies Eqs. (11) and (12) and has the additional property that

$$\langle u_1, v_1|\psi'\rangle = 0. \tag{14}$$

From this it follows that $\psi' \in \mathcal{H}_1^{u_1^\perp} \otimes \mathcal{H}_2^{v_1^\perp}$ and we can repeat the above process on ψ'. Importantly, the dimension of $\mathcal{H}_1^{u_1^\perp} \otimes \mathcal{H}_2^{v_1^\perp}$ is smaller than the dimension of $\mathcal{H}_1 \otimes \mathcal{H}_2$ so this process must terminate. We finally obtain

$$|\psi\rangle = \sum_i M_i|u_i, v_i\rangle, \tag{15}$$

where the sum is over the smaller dimension of $\mathcal{H}_1$ and $\mathcal{H}_2$ and $\{|u_i\rangle\}$ and $\{|v_i\rangle\}$ are orthonormal sets.

For the case where each subsystem has dimensionality 2 we find that

$$|\psi\rangle = M_1|u_1, v_1\rangle + M_2|u_2, v_2\rangle. \tag{16}$$

The phases of M_1 and M_2 can be absorbed into $|u_1, v_1\rangle$ and $|u_2, v_2\rangle$ so we can set them to be real. This decomposition can be written explicitly as

$$\begin{aligned}|\psi\rangle =& \rho^{1/2} e^{i\chi} \left(\cos(\alpha/2) e^{i\tau/2} \begin{pmatrix} \cos(\theta_1/2) e^{-i\phi_1/2} \\ \sin(\theta_1/2) e^{i\phi_1/2} \end{pmatrix} \otimes \begin{pmatrix} \cos(\theta_2/2) e^{-i\phi_2/2} \\ \sin(\theta_2/2) e^{i\phi_2/2} \end{pmatrix} \right. \\ &\left. + \sin(\alpha/2) e^{-i\tau/2} \begin{pmatrix} \sin(\theta_1/2) e^{-i\phi_1/2} \\ -\cos(\theta_1/2) e^{i\phi_1/2} \end{pmatrix} \otimes \begin{pmatrix} \sin(\theta_2/2) e^{-i\phi_2/2} \\ -\cos(\theta_2/2) e^{i\phi_2/2} \end{pmatrix} \right). \end{aligned} \tag{17}$$

This is the Schmidt decomposition for a bipartite 2-state system. In writing this we have satisfied the condition that $\cos\alpha \geq \sin\alpha$ since otherwise $|\langle u_2, v_2|\psi\rangle|^2 > |\langle u_1, v_1|\psi\rangle|^2$ which contradicts our choice of $|u_1, v_1\rangle$.

3.2 The Density Matrix

If we want to calculate expectation values for one particle only and the state of the other particle is unknown then clearly we cannot write down the full wavefunction. We are forced instead to turn to the density operator, $\hat{\rho}$, defined by

$$\hat{\rho} = |\psi\rangle\langle\psi| = \sum_{i,j,k,l} c_{i,j} c^*_{k,l} |i\rangle\langle k| \otimes |j\rangle\langle l| \tag{18}$$

In terms of the density operator the expectation value of any observable $\hat{Q}$ is given by

$$\langle\hat{Q}\rangle = \mathrm{tr}(\hat{\rho}\hat{Q}). \tag{19}$$

The density operator for each particle is given by

$$\hat{\rho}_1 = \mathrm{tr}_2\hat{\rho} = \sum_j \langle j|\hat{\rho}|j\rangle \qquad \hat{\rho}_2 = \mathrm{tr}_1\hat{\rho} = \sum_i \langle i|\hat{\rho}|i\rangle \tag{20}$$

so that the expectation value for the ith particle can be calculated by

$$\langle Q\rangle_i = \mathrm{tr}(\hat{\rho}_i Q). \tag{21}$$

For systems entangled with an (unknown) environment the density matrix represents our ultimate state of knowledge of the system. This has important consequences for the interpretation of quantum mechanics. For a recent review of these ideas, see Paz & Zurek [7].

4 Geometric Algebra

Geometric algebra (GA) is essentially Clifford algebra with added geometric content. Since Clifford algebras are a fundamental part of the treatment of 2-state quantum systems (through the description of quantum spin), we expect

that formulating the theory in a GA framework should bring added geometric insight. This idea was first explored by Hestenes in a series of papers dating back to the sixties [8, 9, 10]. We start by reviewing the treatment of single-particle systems. These are described within the GA of 3D space, denoted $\mathcal{G}_3$. As an orthonormal basis for this we take

$$1, \quad \{\sigma_k\}, \quad \{I\sigma_k\}, \quad I = \sigma_1\sigma_2\sigma_3. \tag{22}$$

The reverse operation (which flips signs of bivectors and trivectors) is denoted with a tilde, and angle brackets $\langle M\rangle_k$ are used to project onto the grade-k part of M. For the projection onto the scalar part we simply write $\langle M\rangle$. For an introduction into the geometric algebra of 3D space see [11, 12].

4.1 Single-Particle Systems

The simplest example of a 2-state system is provided by quantum spin. Spin states can be represented as complex 2-component vectors known as *spinors*. These can be given a more natural encoding within $\mathcal{G}_3$ by defining a linear one-to-one map between the state (as a complex vector) and a multivector constructed from even-grade terms (scalars and bivectors). The simplest such mapping is defined by [2, 3]

$$|\psi\rangle = \begin{pmatrix} a_0 + ia_3 \\ -a_2 + ia_1 \end{pmatrix} \leftrightarrow \psi = a_0 + a_k I\sigma_k, \tag{23}$$

so that the basis elements $|0\rangle$ and $|1\rangle$ map as

$$|0\rangle \leftrightarrow 1 \qquad \text{and} \qquad |1\rangle \leftrightarrow -I\sigma_2. \tag{24}$$

In this way ψ sits inside the space spanned by $\{1, I\sigma_k\}, (k = 1, 2, 3)$. It follows that

$$\psi\tilde{\psi} = (a_0 + a_k I\sigma_k)(a_0 - a_k I\sigma_k) = a_0^2 + a_1^2 + a_2^2 + a_3^2 = \tilde{\psi}\psi \equiv \rho \tag{25}$$

where ρ is the scalar magnitude of the state vector. The multivector ψ can then be written as

$$\psi = \rho^{1/2} R. \tag{26}$$

R is then an even, normalised multivector in 3-dimensions and so is a *rotor* — a generator of rotations.

The action of the Pauli matrices of Eq. (3) is given by

$$\hat{\sigma}_k|\psi\rangle \leftrightarrow \sigma_k\psi\sigma_3 = -I\sigma_k\psi I\sigma_3. \tag{27}$$

It follows that multiplication by i is represented by

$$i|\psi\rangle = \hat{\sigma}_1\hat{\sigma}_2\hat{\sigma}_3|\psi\rangle \leftrightarrow \psi I\sigma_3. \tag{28}$$

To construct observables we define the inner product of two spinors, ψ and ϕ by

$$\langle\psi|\phi\rangle \leftrightarrow (\psi, \phi)_s = \langle\phi\tilde{\psi}\rangle - \langle\phi I\sigma_3\tilde{\psi}\rangle i. \tag{29}$$

As we will see shortly, this definition generalises simply to multiparticle systems. From Eq. (29) the probability density is

$$\langle\psi|\psi\rangle \leftrightarrow (\psi,\psi)_s = \langle\psi\tilde{\psi}\rangle - \langle\psi I\sigma_3\tilde{\psi}\rangle I\sigma_3. \tag{30}$$

But $\psi I\sigma_3\tilde{\psi}$ reverses to give minus itself, so it contains no scalar part. This leaves

$$\langle\psi|\psi\rangle \leftrightarrow (\psi,\psi)_s = \langle\psi\tilde{\psi}\rangle. \tag{31}$$

For the 1-particle case $\psi\tilde{\psi}$ is purely a scalar and is equal to ρ. In the more general case of n-particles we cannot assume that $\psi\tilde{\psi}$ is purely scalar and so Eq. (31), suitably normalised, provides the most general definition for the probability density.

The other observable we can construct is the expectation for the spin in the k-direction. This is given by

$$\begin{aligned}\langle\psi|\sigma_k|\psi\rangle/\langle\psi|\psi\rangle \;&\leftrightarrow \rho^{-1}(\psi,-I\sigma_k\psi I\sigma_3)_s \\ &=\rho^{-1}\langle -I\sigma_k\psi I\sigma_3\tilde{\psi}\rangle - \rho^{-1}\langle -I\sigma_k\psi I\sigma_3 I\sigma_3\tilde{\psi}\rangle I\sigma_3 \\ &=-\rho^{-1}I\sigma_k\cdot\langle\psi I\sigma_3\tilde{\psi}\rangle_2 - \rho^{-1}\langle I\sigma_k\psi\tilde{\psi}\rangle I\sigma_3.\end{aligned} \tag{32}$$

Since $\psi\tilde{\psi}$ is a scalar $\langle I\sigma_k\psi\tilde{\psi}\rangle = 0$. Also, $\psi I\sigma_3\tilde{\psi}$ reverses to give minus itself and has even grade, so is a pure bivector (again in the multiparticle space we cannot make this assumption). Therefore, using Eq. (26) we can define the polarisation bivector by

$$P = \langle\rho^{-1}\psi I\sigma_3\tilde{\psi}\rangle_2 = \langle RI\sigma_3\tilde{R}\rangle_2 \tag{33}$$

so that

$$P_k = \langle\psi|\sigma_k|\psi\rangle/\langle\psi|\psi\rangle = -I\sigma_k\cdot\langle RI\sigma_3\tilde{R}\rangle_2 = -I\sigma_k\cdot P. \tag{34}$$

In this way the spin of the particle can be thought of as a rotation of the $I\sigma_3$ plane, where the rotation is given by the wave function of the particle. The expectation value for the polarisation in the k-direction is then simply the component of P in the k-direction. This was Hestenes' original insight. A challenge is to extend these ideas to the multiparticle framework.

As an example, consider the wavefunction employed in the Schmidt decomposition (17)

$$|\psi\rangle = \begin{pmatrix}\cos(\theta/2)e^{-i\phi/2}\\ \sin(\theta/2)e^{i\phi/2}\end{pmatrix}. \tag{35}$$

In our single particle space this becomes

$$\begin{aligned}\psi &= \cos(\theta/2)e^{-\phi I\sigma_3/2} - \sin(\theta/2)I\sigma_2 e^{\phi I\sigma_3/2} \\ &= e^{-\phi I\sigma_3/2}(\cos(\theta/2) - \sin(\theta/2)I\sigma_2) \\ &= e^{-\phi I\sigma_3/2}e^{-\theta I\sigma_2/2}\end{aligned} \tag{36}$$

and the polarisation vector P is simply

$$\begin{aligned}P = \psi I\sigma_3\tilde{\psi} &= e^{-\phi I\sigma_3/2}e^{-\theta I\sigma_2/2}I\sigma_3 e^{\theta I\sigma_2/2}e^{\phi I\sigma_3/2} \\ &= \sin(\theta)\cos(\phi)I\sigma_1 + \sin(\theta)\sin(\phi)I\sigma_2 + \cos(\theta)I\sigma_3\end{aligned} \tag{37}$$

4.2 2-Particle Systems

States for 2-particle systems are constructed in the multiparticle spacetime algebra (MSTA), which is built from n-particle relativistic configuration space. A basis for this space is provided by the vectors $\{\gamma_\mu^a\}$ where the superscript labels the individual particle space. Vectors from different spaces are orthogonal and so anticommute. It follows that bivectors from different spaces commute, and hence the even subalgebra of the MSTA contains the tensor product of a set of non-relativistic algebras. This is precisely the algebra needed to construct a multiparticle wavefunction. A basis for a 2-particle wavefunction is provided by sums and products of the 1-particle basis elements $\{1, I\sigma_j^1, I\sigma_k^2\}$, where

$$\sigma_k^a = \gamma_k^a \gamma_0^a, \qquad I^a = \gamma_0^a \gamma_1^a \gamma_2^a \gamma_3^a, \qquad \text{(no sum)}. \tag{38}$$

Again, the superscript denotes the particle label, and we abbreviate $I^1\sigma_k^1$ to $I\sigma_k^1$, *etc.*

Currently our basis set gives $4 \times 4 = 16$ real degrees of freedom, whereas we should have only 8 for a 2-particle state. The solution to this problem is to demand a consistent meaning for the unit imaginary. In each separate space multiplication by the imaginary corresponds to right multiplication by $I\sigma_3$. Since our new space has two such bivectors we require that

$$\psi I\sigma_3^1 = \psi I\sigma_3^2, \quad \psi = \psi\tfrac{1}{2}(1 - I\sigma_3^1\, I\sigma_3^2). \tag{39}$$

We therefore define the 2-particle *correlator* [2, 3]

$$E = \tfrac{1}{2}(1 - I\sigma_3^1 I\sigma_3^2), \quad E^2 = E. \tag{40}$$

E is a projection operator and reduces the number of degrees of freedom by a factor of 2. The complex structure in the 2-particle algebra is now defined by the non-simple bivector J, where

$$EI\sigma_3^1 = EI\sigma_3^2 = \tfrac{1}{2}(I\sigma_3^1 + I\sigma_3^2) \equiv J. \tag{41}$$

The two particle spinor $|\psi, \phi\rangle$ is now mapped to the multivector

$$|\psi, \phi\rangle \leftrightarrow \psi^1 \phi^2 E, \tag{42}$$

where the superscripts again denote which space the multivector inhabits. The result of the action of the unit imaginary becomes

$$i|\psi, \phi\rangle \leftrightarrow \psi^1 \phi^2 EI\sigma_3^1 = \psi^1 \phi^2 EI\sigma_3^2 = \psi^1 \phi^2 J. \tag{43}$$

Consistency in this formulation is ensured by the results

$$J^2 = -E \quad \text{and} \quad J = JE = EJ. \tag{44}$$

The action of the individual Pauli matrices now becomes, for example,

$$\hat{\sigma}_k \otimes \hat{I}\,|\psi\rangle \leftrightarrow -I\sigma_k^1 \psi J \tag{45}$$

where $\hat{I}$ is the 2×2 identity matrix. A similar result holds for the second particle space. The action on the right-hand side keeps us in the space of correlated

products of even elements of $\mathcal{G}_3$. The quantum inner product is replaced by the operation

$$\langle\psi|\phi\rangle \leftrightarrow (\psi,\phi)_s = 2\langle\phi E\tilde{\psi}\rangle - 2\langle\phi J\tilde{\psi}\rangle i. \tag{46}$$

The factor of E in the real part is not strictly necessary as it is always present in the spinors, but including it does provide a neat symmetry between the real and imaginary parts. The factor of 2 is included to ensure complete consistency with the standard quantum inner product. (In the general n-particle case a factor of 2^{n-1} is required.)

In Section 3.1 we found that a general 2-particle wavefunction can be written in the form of Eq. (17). To find the geometric algebra form of this we first define the spinor

$$\psi(\theta,\phi) = e^{-\phi I\sigma_3/2}e^{-\theta I\sigma_2/2}. \tag{47}$$

We also need a representation of the orthogonal state to this, which is

$$\begin{aligned}\begin{pmatrix}\sin(\theta/2)e^{-i\phi/2}\\ -\cos(\theta/2)e^{i\phi/2}\end{pmatrix} \leftrightarrow& \sin(\theta/2)e^{-I\sigma_3\phi/2} + \cos(\theta/2)I\sigma_2 e^{I\sigma_3\phi/2}\\ =&\psi(\theta,\phi)I\sigma_2.\end{aligned} \tag{48}$$

It is a straightforward exercise to confirm that this state is orthogonal to $\psi(\theta,\phi)$, as required. We can now construct the MSTA version of the Schmidt decomposition. We replace Eq. (17) with

$$\begin{aligned}\psi =&\rho^{1/2}\Big(\cos(\alpha/2)\psi^1(\theta_1,\phi_1)\psi^2(\theta_2,\phi_2)e^{J\tau/2}\\ &+\sin(\alpha/2)\psi^1(\theta_1,\phi_1)\psi^2(\theta_2,\phi_2)I\sigma_2^1 I\sigma_2^2 e^{-J\tau/2}\Big)e^{J\chi}E\\ =&\rho^{1/2}\psi^1(\theta_1,\phi_1)\psi^2(\theta_2,\phi_2)e^{J\tau/2}\left(\cos(\alpha/2)+\sin(\alpha/2)I\sigma_2^1 I\sigma_2^2\right)e^{J\chi}E.\end{aligned} \tag{49}$$

If we now define the individual rotors

$$R = \psi(\theta_1,\phi_1)e^{I\sigma_3\tau/4}, \quad S = \psi(\theta_2,\phi_2)e^{I\sigma_3\tau/4}, \tag{50}$$

then the wavefunction ψ can be written compactly as

$$\psi = \rho^{1/2}R^1S^2\left(\cos(\alpha/2)+\sin(\alpha/2)I\sigma_2^1 I\sigma_2^2\right)e^{J\chi}E. \tag{51}$$

This gives a neat, general form for an arbitrary 2-particle state. In particular, all reference to the tensor product has been dropped in favour of the somewhat simpler geometric product. The degrees of freedom are held in an overall magnitude and phase, two separate rotors in the individual particle spaces, and a single entanglement angle θ. In total this gives 9 degrees of freedom, so one of them must be redundant. This redundancy is in the single-particle rotors. If we take

$$R \mapsto Re^{I\sigma_3\beta}, \quad S \mapsto Se^{-I\sigma_3\beta} \tag{52}$$

then the overall wavefunction ψ is unchanged. In practice this redundancy is not a problem, and the form of (51) turns out to be extremely useful.

The GA form of the Schmidt decomposition in (51) is very suggestive of a more general pattern. To the left we have rotation operators in each of the individual spaces. In one sense the rotors R^1S^2 can be viewed as representing the nearest direct product (separable) state. Next comes a term describing the 2-particle entanglement. The generalisation seems fairly clear. For a 3-particle system we expect to see terms describing the various 2-particle entanglements, followed by a term for the 3-particle entanglement. Finding precisely the optimal decomposition along these lines is an open problem, but the GA formalism has suggested an approach to the general problem of classifying multiparticle entanglement which has not been tried before.

4.3 2-Particle Observables

We can start to appreciate the utility of the form of (51) by studying the 2-particle observables. These go as, for example

$$\langle\psi|\,\hat{\sigma}_k\otimes\hat{I}\,|\psi\rangle \leftrightarrow (\psi, -I\sigma_k^1\psi J)_s = -2I\sigma_k^1\cdot(\psi J\tilde{\psi}) \tag{53}$$

and

$$\langle\psi|\,\hat{\sigma}_j\otimes\hat{\sigma}_k\,|\psi\rangle \leftrightarrow (\psi, -I\sigma_j^1\, I\sigma_k^2\psi)_s = -2(I\sigma_j^1\, I\sigma_k^2)\cdot(\psi E\tilde{\psi}). \tag{54}$$

All of the observables one can construct are therefore contained in the multivectors $\psi E\tilde{\psi}$ and $\psi J\tilde{\psi}$. This is true in the general n-particle case, and is a major strength of the MSTA approach.

To study the form of the observables we first simplify slightly and set $\rho = 1$. We find that (using $E\tilde{E} = EE = E$)

$$\begin{aligned}\psi E\tilde{\psi} &= R^1S^2\big(\cos(\alpha/2) + \sin(\alpha/2)I\sigma_2^1I\sigma_2^2\big)E \\ &\qquad \big(\cos(\alpha/2) + \sin(\alpha/2)I\sigma_2^1I\sigma_2^2\big)\tilde{R}^1\tilde{S}^2 \\ &= R^1S^2\big(1 + \sin(\alpha)I\sigma_2^1I\sigma_2^2\big)E\tilde{R}^1\tilde{S}^2\end{aligned} \tag{55}$$

Substituting in the form of E from Eq. (40) gives

$$\psi E\tilde{\psi} = \tfrac{1}{2}R^1S^2\Big(1 - I\sigma_3^1I\sigma_3^2 + \sin(\alpha)(I\sigma_2^1I\sigma_2^2 - I\sigma_1^1I\sigma_1^2)\Big)\tilde{R}^1\tilde{S}^2. \tag{56}$$

To make this result clearer we introduce the notation

$$A_k = RI\sigma_k\tilde{R}, \quad B_k = SI\sigma_k\tilde{S} \tag{57}$$

so that

$$\psi E\tilde{\psi} = \tfrac{1}{2}(1 - A_3^1B_3^2) + \tfrac{1}{2}\sin(\alpha)(A_2^1B_2^2 - A_1^1B_1^2). \tag{58}$$

From this we see that

$$\langle\psi E\tilde{\psi}\rangle = \tfrac{1}{2}. \tag{59}$$

This factor of one-half is absorbed by the factor of 2 in the definition of the quantum inner product (46) and shows that the state is correctly normalised to 1. The 4-vector part of the observable is more interesting, as it contains combinations of A_1, A_2, B_1, B_2, none of which are accessible to measurement

in the single-particle case (as they are not phase invariant). This is one place where differences between classical and quantum models of spin start to emerge.

The second observable to form from the 2-particle state ψ is $\psi J\tilde{\psi}$, which is given by

$$\begin{aligned}\psi J\tilde{\psi} &= R^1 S^2\big(\cos(\alpha/2) + \sin(\alpha/2) I\sigma_2^1 I\sigma_2^2\big) J \\ &\qquad \big(\cos(\alpha/2) + \sin(\alpha/2) I\sigma_2^1 I\sigma_2^2\big)\tilde{R}^1\tilde{S}^2 \\ &= \tfrac{1}{2} R^1 S^2\big(\cos^2(\alpha/2) - \sin^2(\alpha/2)\big)(I\sigma_3^1 + I\sigma_3^2)\tilde{R}^1\tilde{S}^2 \\ &= \tfrac{1}{2}\cos(\alpha)(A_3^1 + B_3^2) \end{aligned} \tag{60}$$

This result extends the definition of the polarisation bivector to multiparticle systems. An immediate consequence of this definition is that the lengths of the bivectors are no longer fixed, but instead depend on the entanglement.

4.4 The Density Matrix

The density matrix for a normalised 2-particle pure state can be expanded in terms of products of Pauli matrices as

$$\hat{\rho} = |\psi\rangle\langle\psi| = \frac{1}{4}\big(\hat{I}\otimes\hat{I} + a_k\,\hat{\sigma}_k\otimes\hat{I} + b_k\,\hat{I}\otimes\hat{\sigma}_k + c_{jk}\,\hat{\sigma}_j\otimes\hat{\sigma}_k\big). \tag{61}$$

The various coefficients are found by forming, for example

$$a_k = \langle\psi|\,\hat{\sigma}_k\otimes\hat{I}\,|\psi\rangle = -2I\sigma_k^1\cdot(\psi J\tilde{\psi}) \tag{62}$$

It follows that all of the degrees of freedom present in the density matrix are contained in the multivector observables $\psi E\tilde{\psi}$ and $\psi J\tilde{\psi}$. For mixed states we simply add the weighted values of these observables formed from the pure states. This picture is quite general and works for any number of particles. One small complication is that the terms in $\psi J\tilde{\psi}$ are anti-Hermitian, whereas the density matrix is Hermitian. One way round this is to correlate all of the pseudoscalars together and map all bivectors back to their dual vectors [13] . One can often ignore this feature, however, and work directly with the observables $\psi E\tilde{\psi}$ and $\psi J\tilde{\psi}$.

An advantage of this way of encoding the density matrix is that the partial trace operation to form the reduced density matrix simply consists of throwing away any terms in the observables coming from spaces where the state is unknown. For example, taking the 2-particle entangled state (51) and tracing out the degrees of freedom in space 2 just leaves

$$\hat{\rho} = \tfrac{1}{2}(1 + P_k\hat{\sigma}_k), \quad P_k = (-I\sigma_k)\cdot\big(\cos(\alpha) R I\sigma_3\tilde{R}\big). \tag{63}$$

This shows that the effect of the entanglement is to reduce the expectation value for the polarisation from 1 to $\cos(\alpha)$, but leave the direction of polarisation unchanged. For 2-particle pure states we also see that the polarisation vector is the same length for both particles, so each particle is effected equally by any entanglement which is present. For higher particle number or mixed states the effects of entanglement are more complicated, though the formula

$$P_k = -2^{n-1}(I\sigma_k^a)\cdot(\psi J\tilde{\psi}) \tag{64}$$

holds whenever we form the reduced density matrix for particle a from a larger, entangled state.

Our simple 2-particle system exhibits one of the basic results of quantum theory. When a system entangles with a second, unknown system (usually the environment), the state of the system of interest can no longer be known for certain and we are forced to adopt a density matrix viewpoint. That is, entanglement with the environment leads to decoherence and loss of information.

A useful application of the preceding is to the overlap probability for the inner product of two states. Given two normalised states we have

$$P(\psi,\phi) = |\langle\psi|\phi\rangle|^2 = \mathrm{tr}(\hat{\rho}_\psi\hat{\rho}_\phi). \tag{65}$$

The degrees of freedom in the density matrices are contained in $\psi E\tilde{\psi}$ and $\psi J\tilde{\psi}$, with equivalent expressions for ϕ. One can then show that the probability is given by the compact expression

$$P(\psi,\phi) = \langle(\psi E\tilde{\psi})(\phi E\tilde{\phi})\rangle - \langle(\psi J\tilde{\psi})(\phi J\tilde{\phi})\rangle. \tag{66}$$

This formula holds in the n-particle case as well, except for the presence of an additional factor of 2^{n-2} to give the correct normalisation. This compact expression is a unique feature of the MSTA approach.

As a check on the preceding, suppose we have two separable states

$$\psi = R^1S^2E, \quad \phi = U^1V^2E \tag{67}$$

with

$$\psi E\tilde{\psi} = \tfrac{1}{2}(1 - A^1B^2), \quad \phi E\tilde{\phi} = \tfrac{1}{2}(1 - C^1D^2). \tag{68}$$

We find that

$$\begin{aligned} P(\psi,\phi) &= \tfrac{1}{4}\langle(1 - A^1B^2)(1 - C^1D^2) - (A^1 + B^2)(C^1 + D^2)\rangle \\ &= \tfrac{1}{4}(1 + A\cdot C\, B\cdot D - A\cdot C - B\cdot D) \\ &= \tfrac{1}{2}(1 - A\cdot C)\,\tfrac{1}{2}(1 - B\cdot D) \end{aligned} \tag{69}$$

which shows that the probability is the product of the separate single-particle probabilities. If one of the states is entangled this result no longer holds.

4.5 Example – The Singlet State

As a simple example of the some of the preceding ideas, consider the spin-singlet state

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle) \leftrightarrow \psi = \frac{1}{\sqrt{2}}(I\sigma_2^1 - I\sigma_2^2)E. \tag{70}$$

This state is maximally entangled ($\alpha = \pi/2$), and isotropic. Forming the two observables we find that

$$\psi E\tilde{\psi} = \tfrac{1}{2}(1 + I\sigma_k^1\, I\sigma_k^2) \tag{71}$$

and

$$\psi J\tilde{\psi} = 0. \tag{72}$$

It follows that the reduced density matrix for either particle space is simply one-half of the identity matrix, and so all directions are equally likely. If we align our measuring apparatus along some given axis and measure the state of particle one then both up and down have equal probabilities of one-half.

Suppose now that we construct a joint measurement on the singlet state. We can model this as the overlap probability between ψ and the separable state

$$\phi = R^1 S^2 E. \tag{73}$$

Denoting the spin directions by

$$RI\sigma_3\tilde{R} = P, \quad SI\sigma_3\tilde{S} = Q, \tag{74}$$

we find that, from (66)

$$\begin{aligned} P(\psi,\phi) &= \langle \tfrac{1}{2}(1 - P^1 Q^2)\tfrac{1}{2}(1 + I\sigma_k^1\, I\sigma_k^2)\rangle \\ &= \tfrac{1}{4}(1 - P\cdot(I\sigma_k)\, Q\cdot(I\sigma_k)) \\ &= \tfrac{1}{4}(1 - \cos\theta) \end{aligned} \tag{75}$$

where θ is the angle between the spin bivectors P and Q. So, for example, the probability that both measurements result in the particles having the same spin ($\theta = 0$) is zero, as expected. Similarly, if the measuring devices are aligned, the probability that particle one is up and particle two is down is one-half, whereas if there was no entanglement we should get the product of the separate single particle measurements (resulting in 1/4).

It is instructive to see how all of strange quantum entanglement results for the singlet state are contained in the 4-vector part of the observables. This reveals some of the complex geometry associated with multiparticle quantum mechanics. And this is only for 2-particle systems! Most proposals for quantum computers have in mind a far greater number of entangled qubits. We hope that this paper has demonstrated some of the potential power of geometric algebra for helping to navigate through these large Hilbert spaces.

5 Acknowledgements

Rachel Parker is supported by the Cambridge Commonwealth Trust and the Kerry Packer Scholarship Foundation. Chris Doran is supported by the EPSRC. The authors thank Anthony Lasenby and Timothy Havel for helpful discussions.

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