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Electron Configuration and Quantum Entanglement

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Abstract: With the advent of general relativity and quantum mechanics, physics has in many cases shifted the emphasis from dynamics to symmetry principles associated with different types of mathematical groups. We speak of the group structure of crystals, the group invariants of the equations of motion, the group classification of elementary particles, and also of the group homeomorphisms of fractals. The objective of this article is to show how the group theoretical structure of entanglement can be used to classify atomic and molecular structure. The article begins by establishing a working definition of entanglement and then using it to derive the Pauli-exclusion principle by showing that Fermi-Dirac statistics can be considered as an entangled state invariant under the action of the $SL(n, C)$ group. Based on this, a group classification scheme of entangled states is proposed to distinguish atomic and molecular structures associated with chemical bonds.

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1. Introduction

Quantum entanglement is not an easy phenomenon to grasp. It involves both an understanding of probability and statistics, a distinction between pure and mixed states, the difference between indistinguishable and distinguishable states, an appreciation of L^2 functions and a knowledge of group theory (which is often overlooked). Moreover, any serious dicussion of the topic requires the use of a mathematical definition, and it is not always clear that it coincides fully with the physics understanding of the phenomenon. Whereas most papers on the topic of entanglement dwell upon the notions of "locality" and "non-locality", entropy, Bell's inequality and variations thereof [1], this paper is comparatively unique it that it focuses on the group theoretical properties of entangled states, associated with "the information in a composite system [that] resides more in the correlations than in properties of individuals." [1] This contrasts with other articles, where group theory, if mentioned, is only associated with a "covariant representation of spin and entanglement", [2] or with the "appropriate way to interpret the covariant entropy bound" [3]. Instead, we classifiy entangled states using group theory, and in particular show that there is a form of entanglement associated with the Bell states that distinguishes "bonding orbitals" from "antibonding orbitals" and also Fermi-Dirac and Bose-Einstein statistics, which in turn can be used to further classify atomic and molecular structure. Before presenting a rigorous definition, we explore the meaning of entanglement from an intuitive point of view.

Imagine two people looking downwards, one at the north pole and the other at the south. Each is asked to denote their downward direction with a vector. Both would probably write $|\downarrow\rangle$. However, if a neutral observer attempts to characterize the "looking down," s/he will notice that the two vectors are in opposite directions relative to one another, and can be represented by either $|\downarrow\uparrow\rangle$ or $|\uparrow\downarrow\rangle$, depending on which convention is chosen to represent north and south. Moreover, if north and south are replaced by any two diametrically opposite positions on the sphere, the same dilemma arises. The words "up" and "down" are interchangeable and rotationally invariant in that they apply to any diametrically opposite positions on the sphere. "Looking down" loses meaning in the sense what is "down" for one observer is "up" for the other and vice-versa.They are indistinguisable. In this case, it would be better to represent the two states by the vector $\frac{1}{2}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ or $\frac{1}{2}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$, where the $\frac{1}{2}$ indicates that each representation has equal weighting.

In other words, "up" and "down" have no absolute meaning, although the two vectors must point in opposite directions. For this reason, the latter two representations can be considered more realistic in that they represent a superposition of two possibilities $|\downarrow\uparrow\rangle$ or $|\uparrow\downarrow\rangle$ and do not give preference to one representation over another, or to one direction over another. This becomes even more pronounced at the quantum level, where the two states are indistinguishable from one another, meaning that one cannot observe in principle "up" or "down" "left" or "right" without disturbing the system. The act of observation usually forces us to impose a preferred reference frame and it doing so breaks the superposition. Also, the mathematical framework of quantum mechanics is formulated in terms of a Hilbert space and in this case it is preferable to write the superposed state as

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)\,, \tag{1}$$

where $\frac{1}{\sqrt{2}}$ corresponds to the amplitude of the state vector and its square, $\frac{1}{2}$, to the respective probability weightings. We could also agree to write it as

$$\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)\,. \tag{2}$$

The choice is ours. Indeed, someone could argue that it is better to write the joint superposed state as

$$\frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)\,, \tag{3}$$

where the $\uparrow\uparrow$ corresponds to both of them "looking up" or $\downarrow\downarrow$ corresponds to both "looking down" depending on ones point of view. Either way, whether we use (1), (2) or (3) each represents an entangled state. As we will show later, all of these states are rotationally invariant in that they all represent "looking down" (or "looking up") from any arbitrary positions on the globe provided they are diametrically opposite.

In many cases, including all rotationally invariant states, the entangled state is by definition a superposition of two indistinguishable states and if an experiment is carried out to distinguish one from the other, it means that the entanglement has been broken. Mathematically speaking, we could say that the wavefunction has collapsed. For example in the case of (1), a measurement will cause $|\psi\rangle$ to transition into either the state $|\uparrow\downarrow\rangle$ or $|\downarrow\uparrow\rangle$. Usually in quantum mechanics this is referred to as collapsing the wave function, and in effect, it means that we have transitioned from a superposed state to a separable or factored state.

Secondly, it is common practice to distinguish a pure (including pure entangled) state from mixed and unentangled states by means of the density matrix[1], which is defined as the outer product of the original states. With this in mind, we change notation and replace $|\uparrow\rangle$ and $|\downarrow\rangle$ by $|+\rangle$ and $|-\rangle$ respectively, with the understanding that $|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. Now consider the state

$$|\psi\rangle = p|+\rangle + q|-\rangle \tag{4}$$

then the density function ρ_1 is defined to be

$$\begin{aligned} \rho_1 &= |\psi\rangle\langle\psi| \\ &= \begin{pmatrix} p^2 & pq^* \\ p^*q & q^2 \end{pmatrix},\ p^2 + q^2 = 1 \end{aligned}$$

[1] The density matrix seems to have been first introduced to quantum mechanics by von Neumann [4] and as noted by Tolman [5] the components ρ_{nm} of a density matrix “play a role somewhat similar to that of the density ρ in the classical mechanics”

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Note that $\rho_1^2 = \rho_1$ in this case. If the wave function has collapsed, it means that the linear superposition has been broken and that it has been reduced to either the pure $|+\rangle$ or $|-\rangle$ with probabilities p^2 and q^2 respectively.

We can also define a density function that represents the probability ensemble of two states:

$$\begin{aligned} \rho_2 &= p^2|+\rangle\langle+| + q^2|-\rangle\langle-| \\ &= \begin{pmatrix} p^2 & 0 \\ 0 & q^2 \end{pmatrix}, \; p^2 + q^2 = 1 \end{aligned}$$

They can be interpreted as an ensemble of two separable states, usually associated with identical particles. Sometimes ρ_2 is referred to as a density matrix of mixed states. The transitions from $\rho_1 \to \rho_2$ occurs experimentally when we assign proability weightings to the collapsed wave functions or more precisely to the probability distribution of mutually exclusive events.

A third point to note is that equation (4) could also have been writen as

$$|\tilde{\psi}\rangle = p|+-\rangle + q|-+\rangle \tag{5}$$

corresponding to the fact that "up or down" at one pole can be simultaneously interpreteted as "down or up" at the other pole. It is analogous to flipping a coin. If we observe that a "head" is up then simultaneously we know that a "tail" is down. One observation implicitly implies two pieces of information. This is also carried over into the density matrix for the superposed state (6) below, which is given by

$$\begin{aligned} \tilde{\rho}_1 &= |\tilde{\psi}\rangle\langle\tilde{\psi}| \\ &= (p|+\rangle|-\rangle + q|-\rangle|+\rangle)(p^*\langle+|\langle-| + q^*\langle-\rangle\langle+|) \\ &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & p^2 & pq^* & 0 \\ 0 & p^*q & q^2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \; p^2 + q^2 = 1 \end{aligned}$$

It essentially carries the same information as ρ_1. Note that $\tilde{\rho}_1^2 = \tilde{\rho}_1$, $tr(\tilde{\rho}_1) = tr(\rho_1)$, $det(\rho_1) = det(\tilde{\rho}_1)$ and there is a clear bijection between $\tilde{\rho}_1 \leftrightarrow \rho_1$. In other words, the previous comment that one observation yields two pieces of information carries over into density matrices.

Fourtly, this brings us to an important point regarding the principle of microcausality. Since an entangled (singlet) state simultaneously permits two pieces of information to be obtained from one measurement, the principle of microcausality is violated in this case. Nonlocal events violate microcausality by definition. In does not mean that a physical signal is transmitted faster (or indeed slower) than the speed of light. It is the ontological observation that one measurement yields two pieces of information. In the case of a regular coin if the head (H) is "up" then simultaneously we know the tail (T) is "down". The same applies to spin-singlet states (see equation (2)). When, the spin value of one particle is measured then simultaneoulsly the spin value of the other particle is known. This has serious implications for the spin-statistics theorem [6] and will be discussed in more detail in Section 3.2.

2. Theoretical Requirements and Methods

2.1. A Working Definition of Entanglement

Definition 1. *Let $\mathcal{H}_1, \ldots \mathcal{H}_k$ be k (n-dimensional) Hilbert spaces such that $k \le n$. Let*

$$|\psi(x_1, x_2, \ldots, x_k)\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2 \cdots \otimes \mathcal{H}_k.$$

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If there exist a set of states $|\psi\rangle_i \in \mathcal{H}_i$ *such that*

$$|\psi(x_1, x_2, \ldots x_k)\rangle = |\psi\rangle_1 \otimes |\psi\rangle_2 \cdots \otimes |\psi\rangle_k$$

then $|\psi(x_1, x_2, \ldots, x_k)\rangle$ *is* **not** *entangled. Otherwise it is said to be entangled.*

This definition is in agreement with [7,8]. The entangled states can be further subdivided into fully entangled states, which cannot be factored over $\mathcal{H}_1, \ldots \mathcal{H}_k$ and partially entangled states, which can be partially factored over $\mathcal{H}_1, \ldots \mathcal{H}_k$. For example, if $\mathcal{H}_1 = \mathcal{H}_2 = \mathcal{H}$ and $|+\rangle \in \mathcal{H}$ and $|-\rangle \in \mathcal{H}$ are orthogonal vectors then $|+\rangle|+\rangle$ and $|+\rangle|-\rangle$ are (pure) unentangled states, with respective density matrices given by

$$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \text{ and } \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

and the corresponding mixed density matrix is given by ρ_2 (equation (5)). In contrast, the entangled state $|\psi\rangle = \frac{1}{\sqrt{2}}(|+\rangle|-\rangle - |-\rangle|+\rangle)$ is represented by the density matrix ρ_1.

As another example consider the tensor product $\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3$ then

1. $|\psi\rangle_1 \otimes |\psi\rangle_2 \otimes |\psi\rangle_3 + |\psi\rangle_2 \otimes |\psi\rangle_3 \otimes |\psi\rangle_1 + |\psi\rangle_3 \otimes |\psi\rangle_1 \otimes |\psi\rangle_2$ is entangled
2. $|\psi\rangle_1 \otimes (|\psi\rangle_2 \otimes |\psi\rangle_3 + |\psi\rangle_3 \otimes |\psi\rangle_2)$ is a partially entangled state.
3. $|\psi\rangle_1 \otimes |\psi\rangle_2 \otimes |\psi\rangle_3$ as a factored state is not entangled.

We have already noted in the introduction that many cases of entanglement can be associated with some degree of indistinguishability, although there are indistinguishable states that are not entangled (see triplet state defined below) and the mathematical definition does not per se refer to indistinguishability. In general, given $\mathcal{H} = \mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_k$ then $|\psi\rangle \in \mathcal{H}$ is entangled if it can be written as a non-separable orthonormal state

$$|\psi\rangle = \sum c_{i_1 \ldots i_k} |\psi\rangle_{i_1} \otimes \cdots \otimes |\psi\rangle_{i_k}, \; c_{i_1 \ldots i_k} \neq 0 \text{ or } \neq 1$$

This is strictly a mathematical definition and it remains an open question whether all such states are realizable in nature and whether such a definition truly captures the essence of entanglement as it occurs in physics. The previously defined set of states $|\psi\rangle_i$ can be combined to form a linear combination of $k!$ terms, if $|\psi\rangle_i \neq |\psi\rangle_j$ for $i \neq j$. Moreover, if each $|c_i|$ are equal for all i then the state $|\psi\rangle$ is indistinguishable, meaning that it is invariant under the action of a permutation group S_n, where n correponds to the number of non-zero c_i terms. For example, if $k = 2$, the state

$$|\psi\rangle = c_{11}|++\rangle_1 + c_{12}|+-\rangle + c_{21}|-+\rangle + c_{22}|--\rangle, \; c_{11}^2 + c_{12}^2 + c_{21}^2 + c_{22}^2 = 1\,,$$

is entangled provided the c_i are chosen so as $|\psi\rangle$ is not factorable. Indeed, $c_{11}^2 = c_{12}^2 = c_{21}^2 = c_{22}^2 = \frac{1}{4}$ defines an unentangled triplet state

$$\frac{1}{2}(|+\rangle + |-\rangle) \otimes (|+\rangle + |-\rangle)\,. \tag{6}$$

The triplet state serves as a good example to how mathematical and physical models may differ. Mathematically speaking there are two ways to look at this. Either we view it as a tensor product of two states (or qubits), each of which is a linear superposition of $|+\rangle$ and $|-\rangle$, and write this product as

$$|\psi\rangle = \frac{1}{2}|++\rangle + \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}(|+-\rangle + |-+\rangle)\right) + \frac{1}{2}|--\rangle \tag{7}$$

$$= \frac{1}{2}|1\rangle + \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{2}|-1\rangle \tag{8}$$

with the understanding that $|1\rangle = |{+}{+}\rangle$, $|0\rangle = (\frac{1}{\sqrt{2}}(|{+}{-}\rangle + |{-}{+}\rangle)$ and $|{-1}\rangle = |{-}{-}\rangle$ with respective probability weightings of $\{1/4, 1/2, 1/4\}$ or we view it as a superposition of three unit vectors $|{-1}\rangle, |0\rangle, |1\rangle$ defined over a three dimensional vector space with respective probability weightings of $\{1/3, 1/3, 1/3\}$. Many physicists believe that the latter is the correct answer. The author of this article believes that a spin 1 state will have the probability decomposition $\{1/4, 1/2, 1/4\}$, given that the spin 1 state of atoms and mesons (composed of two quarks) arises from the presence of two spin 1/2-particles. The final answer will depend on experiment. Either way, the triplet state is **not** rotationally invariant.

In the case of a bivector composed of two orthogonal vectors, this reduces to a maximally entangled state of the form

$$|\psi\rangle = c_{12}|{+}{-}\rangle + c_{21}|{-}{+}\rangle,\ c_{12}^2 + c_{21}^2 = 1$$

which in turn reduces to a singlet state

$$\frac{1}{\sqrt{2}}(|{+}{-}\rangle - |{-}{+}\rangle)$$

when $c_{12}^2 = c_{21}^2 = \frac{1}{2}$.

It should be immediately noted that each $c_{i_1 \ldots i_k}$ can be either posivive or negative and consequently by associating a probability measure with the L^2 property of $|\psi\rangle$, many of the usual properties of probability spaces are no longer valid [4] as is the case with the Chapman-Kolmogorov equations [9].

2.2. Bell States

The Bell states are defined as follows [8]:

$$|\psi\rangle_1 = \frac{1}{\sqrt{2}}(|+\rangle|+\rangle + |-\rangle|-\rangle) \quad (9)$$

$$|\psi\rangle_2 = \frac{1}{\sqrt{2}}(|+\rangle|-\rangle - |-\rangle|+\rangle) \quad (10)$$

$$|\psi\rangle_3 = \frac{1}{\sqrt{2}}(|+\rangle|+\rangle - |-\rangle|-\rangle) \quad (11)$$

$$|\psi\rangle_4 = \frac{1}{\sqrt{2}}(|+\rangle|-\rangle + |-\rangle|+\rangle) \quad (12)$$

First note that the set $\{|\psi\rangle_1, |\psi\rangle_2\}$ is composed of conjugate spinors[2] as also is the set $\{|\psi\rangle_3, |\psi\rangle_4\}$. Secondly, all four Bell states subdivide into two sets of rotationally invariant states. In other words, $(R,R)|\psi\rangle_1 = |\psi\rangle_1$ and $(R,R)|\psi\rangle_2 = |\psi\rangle_2$, while $(R,R^T)|\psi\rangle_3 = |\psi\rangle_3$ and $(R,R^T)|\psi\rangle_4 = |\psi\rangle_4$. In general, letting $|\psi\rangle = |\psi\rangle_1 + |\psi\rangle_2$ and $|\phi\rangle = |\psi\rangle_3 + |\psi\rangle_4$, it follows that

$$(R,R)|\psi\rangle = (R,R)|\psi\rangle_1 + (R,R)|\psi\rangle_2 = |\psi\rangle$$

and

$$(R,R^T)|\phi\rangle = (R,R^T)|\psi\rangle_3 + (R,R^T)|\psi\rangle_4 = |\phi\rangle\ .$$

Moreover, we note that the state

$$\frac{1}{\sqrt{2}}(|\psi\rangle_1 + |\psi\rangle_4) = \frac{1}{2}(|+\rangle|+\rangle + |-\rangle|-\rangle + |+\rangle|-\rangle + |-\rangle|+\rangle) \quad (13)$$

$$= \frac{1}{2}(|+\rangle + |-\rangle) \otimes (|+\rangle + |-\rangle) \quad (14)$$

[2] Some textbooks refer to $i|\psi\rangle_2$ and $i|\psi\rangle_4$ as the conjugate spinors. For the purpose of this article, we drop the $i = \sqrt{-1}$ for convenience because it substantially makes no difference.

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is factorable over a subspace of the tesor product space $H_1 \otimes H_2$. It is not rotationally invariant, and its probability density function is given by

$$\rho = \frac{1}{4}(|+\rangle + |-\rangle) \otimes (|+\rangle + |-\rangle)((\langle +| + \langle -|) \otimes ((\langle +| + \langle -|) \tag{15}$$

$$= \frac{1}{4}\left[\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}\right] \tag{16}$$

The reduced density functions are given by

$$\rho_1 = \rho_2 = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$$

Therefore, $Tr(\rho_1) = Tr(\rho_2) = 1$ and the von Neumann entropy [4] $Tr(\rho_1 \ln(\rho_1) = Tr(\rho_2 \ln \rho_2) = 0$. This means that the entropy of each subsystem is 0.

Again, if we consider the state

$$\frac{1}{\sqrt{2}}(|\psi\rangle_1 + i|\psi\rangle_2) = \frac{1}{2}(|+\rangle|+\rangle + |-\rangle|-\rangle + i|+\rangle|-\rangle - i|-\rangle|+\rangle) \tag{17}$$

$$= \frac{1}{2}(|+\rangle - i|-\rangle) \otimes (|+\rangle + i|-\rangle) \tag{18}$$

In contrast to equation (13), this state is rotationally invariant, the trace of each subsystem is 1 and their entropy is 0. However, if we consider the state $\frac{1}{\sqrt{2}}(|\psi\rangle_1 + |\psi\rangle_2)$, it is not factorable but it is rotationally invariant. Consequently, we find that both of the states $\frac{1}{\sqrt{2}}(|\psi\rangle_1 + |\psi\rangle_4)$ and $\frac{1}{\sqrt{2}}(|\psi\rangle_1 + i|\psi\rangle_2)$ have entropy 0, but in contrast the state $\frac{1}{\sqrt{2}}(|\psi\rangle_1 + i|\psi\rangle_2)$ is rotational invariant, while the state $\frac{1}{\sqrt{2}}(|\psi\rangle_1 + |\psi\rangle_4)$ is not. Also, $\frac{1}{\sqrt{2}}(|\psi\rangle_1 + |\psi\rangle_2)$ has a positive entropy and it is also rotationally invariant. In other words, neither entropy alone nor rotational invariance alone are sufficient to distinguish between the different types of entangled and unentangled states. Something more is needed.

2.3. Isotropically Spin Correlated States

All four Bell states considered individually are not only rotationally invariant but also isotropically spin correlated (ISC) [10,11].

Definition 2. *More formally n (quantum) particles are said to be isotropically spin-correlated (ISC), if a measurement made in an arbitrary direction on one of the particles allows us to predict with certainty the spin value of each of the other $n-1$ particles for the same direction.*

For example, if two photons are in a singlet state then no matter the orientaion of the polarizer, the two photons will always be in equal and opposite polarized states. A singlet state means that the photons are polarized in every direction at once. There is no preferred direction. It is only by passing the individual photons through a polarizer that we impose a specific polarization. The same principle also holds for electrons in a spin-singlet state. There is no preferred direction. A measurement of spin value in an arbitrary direction will simultaneously yield an equal and opposite value for the other electron. The same logic also applies to all four Bell states. In the case of $|\psi\rangle_1$ the rotational invariance means that if we measure one value in an arbitrary direction in the plane then the other partcle will have the same value if it were measured in the same direction. One might think of the state $|\psi\rangle_1$ as corresponding to parallel molecular bonding in chemistry and $|\psi\rangle_2$ corresponding to anti-parallel molecular bonds.

It is not immediately clear that ISC states must occur in pairs, which gives a privileged position to the four Bell states in that they may be considered the building blocks of all entangled systems. For example, one could mathematically define a state

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|+\rangle|+\rangle|+\rangle + |-\rangle|-\rangle|-\rangle)$$

This is a special case of equation (30) below. As written, it seems to correspond to three ISC (quantum) particles in that an observation of the state of a single particle collapses the wave function into either $|+\rangle|+\rangle|+\rangle$ or $|-\rangle|-\rangle|-\rangle$, which means that one observation yields three pieces of information. However, as it turns out $|\psi\rangle$ is not rotationally invariant and unlike the Bell states defined above $|\psi\rangle$ is not isotropic. It represents a polarized state in a specified direction or in three different directions but not in an arbitrary direction. It is an example of GHZ state. A more detailed discussion of this can be found in Section 8.

To better understand this intuitively, consider by way of analogy that the "spin-up" and "spin-down" observables associated with a singlet state correspond to a right and left hand respectively. In the case of $|\psi\rangle$, there is no reason we cannot draw three identical right hands and three identical left hands. We first draw one hand, and then can repeat the process ad infinitum to draw as many identical hands as we wish. We could say that the parameters that permit us to draw one right hand can be used over and over again to draw a second and then a third and so on, The same can be done with the left hand if needed. Using the same logic, one might expect that if we know all the parameters associated with determining the spin of an electron then we could repeat the same procedure to produce n identical electrons. Einstein believed such parameters existed ([4], p. 209, [12,13]) and that quantum mechnics as formulated was a mere cloak for ignorance and led "to spooky action at a distance." As it turns out, because of Bell's inequality [14] there are no hidden parameters and therefore spin states cannot be cloned. In other words, the analogy does not work. There are no hidden paprameters that allow us to duplicate the isotropic properties of spin. Nature allows for mirror images (parity if you like) but it does not rely on hidden variables to create the mirror image. This leads to the following theorem

Theorem 1. *$|\psi_1\rangle$ and $|\psi_2\rangle$ are the only ISC states up to isomorphism.*

A proof based on Bell's inequality is given in [9,10]. The argument essentially runs as follows: if three (or more) ISC particles existed then one could observe three ISC states, one on each particle, in three different and independent directions because of the pairwise rotational invariance. The probability structure of these three observations can be related by Bell's inequality resulting in a mathematical contradiction. Since, nature does not allow for such contradictions, we conclude that three or more ISC particles do not exist. Note that no contradiction arises in the case of two ISC states.

Indeed the set $\{|\psi\rangle_1, |\psi\rangle_2\}$ as conjugate spinors represents parallel and anti-parallel pairing respectively. The theory can also be formulated in terms of $\{|\psi\rangle_3, |\psi\rangle_4\}$. As noted in [11]: "there is a duality principle at work which defines a $1 \leftrightarrow 1$ relation between the Hilbert spaces spanned by $\{|\psi\rangle_1, |\psi\rangle_2\}$ and $\{|\psi\rangle_3, |\psi\rangle_4\}$. For example, if we were to define ISC states in terms of invariance under $R(\theta) \otimes R^T(\theta)$ then by duality, we could apply Theorem 1 to $|\psi\rangle_3$, $|\psi\rangle_4$." In this article we will work primarily with $|\psi\rangle_1$ and $|\psi\rangle_2$.

As Definition 1 shows, mathematically speaking there are many possible entangled states. However, in practise when considering the world of physics, there is overwhelming evidence both from the theory of superconductors and molecular bonding theory that nature priveleges pairwise ISC entangled states [15–32]. Moreover, as we have noted here and elsewhere, the Pauli exclusion principle can be proven by assuming the existence of indistinguishable ISC pairs or equivalently the Bell states. For this reason, we claim that ISC states are in many ways the building blocks of entanglement as it occurs in nature. In the light of theorem 1, we can **redefine** an orbital as follows:

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Definition 3. *Two particles are in the same orbital if their joint spin forms a Bell state.*

In the case of atomic and molecular bonds, these orbitals can be further distinguised by specifying the n, l, m quantum numbers associated with energy, angular momnetum and the z component of angular momentum.

2.4. A Clifford Algebra of Entangled States

The cojugate pair $\{|\psi\rangle_1, |\psi\rangle_2\}$ or $\{|\psi\rangle_3, |\psi\rangle_4\}$ in addition to being rotationally invariant also define a basis for a Clifford algebra. This means that in the case of a bivariate system, all rotationally invariant states are constructed from the four ISC Bell states, which can be further subdivided into two disjoint Hilbert subspaces of $\mathcal{H}_1 \otimes \mathcal{H}_2$. Specifically, there exists a Hilbert space $\mathcal{H}_{12} \subset \mathcal{H}_1 \otimes \mathcal{H}_2$ with $X, Y \in \mathcal{H}$ such that $XY \in \mathcal{H}_{12}$ if and only if

$$XY \equiv \langle X, Y\rangle_{\otimes} + [X, Y]_{\otimes} \tag{19}$$

defines a Clifford Algebra[3] with respect to the basis $\{|\psi\rangle_1, |\psi\rangle_2\}$, with the understanding that

$$\begin{aligned} \langle X, Y\rangle_{\otimes} &\equiv X \otimes Y + Y^{\perp} \otimes X^{\perp} &(20)\\ &= (x_1 y_1 + x_2 y_2)(|+\rangle|+\rangle + |-\rangle|-\rangle) &(21)\end{aligned}$$

defines an inner product and

$$\begin{aligned} [X, Y]_{\otimes} &\equiv X \otimes Y - Y \otimes X &(22)\\ &= (x_1 y_2 - x_2 y_1)(|+\rangle|-\rangle - |-\rangle|+\rangle) &(23)\end{aligned}$$

defines an outer product. Note that the Clifford Algebra is rotationally invariant with respect to $R \otimes R$. Indeed, in the case of a bivariate set of vectors the above set of relationships can be identified with the complex numbers. To see this, consider $z_1, z_2 \in \mathcal{C}$ then

$$\bar{z}_1 z_2 = (x_1 - i y_1)(x_2 + i y_2) = x_1 x_2 + y_1 y_2 + i(x_1 y_2 - x_2 y_1) \tag{24}$$

and note that $Re(\bar{z}_1 z_2) = \langle X, Y\rangle_{\otimes}$ and $Im(\bar{z}_1 z_2) = [X, Y]_{\otimes}$

Similarly the dual basis $\{|\psi\rangle_3, |\psi\rangle_4\}$ can be used to define a conjugate Clifford algebra over a Hilbert space $\mathcal{H}_{34}$ given by

$$XY \equiv \langle X, Y\rangle_d + (X \wedge Y)_d \tag{25}$$

with respect to the basis $\{|\psi\rangle_3, |\psi\rangle_4\}$, with the understanding that $X = (x_1, i x_2)$, $X^c = (x_1, -i x_2)$ and $\tilde{X} = (i x_2, x_1)$ such that

$$\begin{aligned} \langle X, Y\rangle_d &\equiv X \otimes Y - \tilde{Y} \otimes \tilde{X} &(26)\\ &= (x_1 y_1 + x_2 y_2)(|+\rangle|+\rangle - |-\rangle|-\rangle) &(27)\end{aligned}$$

defines an inner product and

$$\begin{aligned} X \wedge Y &\equiv X^c \otimes Y - Y^c \otimes X &(28)\\ &= (x_1 y_2 - x_2 y_1)(|+\rangle|-\rangle + |-\rangle|+\rangle) &(29)\end{aligned}$$

an outer product. The conjugate Clifford Algebra is rotational invariant under the action of $R \otimes R^T$.

Since the two Hilbert spaces $\mathcal{H}_{12}, \mathcal{H}_{34}$ are isomorphic to each other under conjugation, for the remainder of this article we will work with the space $\mathcal{H}_{12}$. We note that the wedge product or the Lie product of the Clifford algebra $[X, Y]_{\otimes}$ is invariant under the action of $SL(2, \mathcal{C})$ group and corresonds

[3] A description of the use of Clifford Algebra in physics can be found in [33]

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to a bivector. Note that the $SL(2,\mathcal{C})$ can be represented by the set of 2×2 matrices over the complex numbers with determinant 1.

3. Results

3.1. Molecular Bonding

The existence of such paired ISC states raises an interesting question regarding the best classification of entantagled states especially in multivariate systems composed of molecules. In general chemistry a "bonding orbital" is produced when the energy of the molecular orbital is lower that the sum of the two individual orbitals from which it was composed. For example, when the electrons of two hydrogen atoms bind to form a molecular orbital bond of H_2 with spin state $|\psi\rangle_2$ it corresponds to the constructive interference of overlapping wave functions of the individual electrons, encapsulated by the singlet state with total spin 0. Consequently, the singlet has a lower energy than the sum of the two components taken separately. In contrast, an "antibonding orbital" occurs when the wave functions overlap out of phase (destructive interference) to produce a spin state $|\psi\rangle_1$. In this case, the bonding energy is higher than the sum of the individual energies associated with each separate state. Moreover, given that the spin states of $|\psi\rangle_1$ are parallel to each other, one can anticipate that this type of bond will have paramagnetic effects, while those of $|\psi\rangle_2$ will be diamagnetic. For the purpose of this article, we denote the molecular orbitals of the ISC states $|\psi\rangle_1$ and $|\psi\rangle_2$ by σ^* and σ respectively. However, this differs from the usual use of the language in chemistry.

For example, in traditional molecular bonding theory the molecule Li_2 will have the electron decomposition $\sigma_{1s}, \sigma^*_{1s}, \sigma_{2s}$, whereas in this new formulation it would be given by $2\sigma_{1s}, \sigma_{2s}$ where the $2\sigma_{1s}$ recognizes that there is σ_{1s} orbital associated with each atom, which one would also expect from symmetry, while the σ_{2s} refers to the shared molecular orbital. Overall the new notation indicates that there exists three spin-singlet states, each of which can be represented by $|\psi\rangle_2$.

As a second example, we consider the boron molecule B_2. Traditional molecular orbital theory lists the orbital structure as $\sigma_{1s}, \sigma^*_{1s}, \sigma_{2s}, \sigma^*_{2s}, \pi_{2p_y}, \pi_{2p_z}$ where the π_{2p_y}, π_{2p_z} are refered to as unpaired electrons with parallel spins. In the new representation we write $2\sigma_{1s}, 2\sigma_{2s}, \sigma^*_{2p}$ for the electron configuration. The presence of σ^*_{2p} also indicates the presence of paramagnetism and the overall formulation respects the symmetry of B_2.

In general, the transition from two non-interacting electrons to interacting electrons by means of the chemical reaction, can be considered as a phase transition from the triplet state (cf equations (6-8)) to the rotationally invariant Clifford algebra state given by equation (19), which in turn transitions to an equilibrium ISC state given by equations (21) and (23), which form an orthnormal basis for the Clifford algebra. This transition from the Clifford state to one of the ISC states is mediated by the rule of "maximum multiplicity and minimal energy." In fact, a spin-singlet state represented by $|\psi\rangle_2$ might be expected to exhibit diamagnetic properties while those in the parallel state represented by $|\psi\rangle_1$ might be expected to exhibit paramagnetism. The intensity of these effects will depend upon the physical closeness of the ISC states. As numerous experiments have demonstrated, the existence of ISC states are related to non-locality and can exist both over short-range and long-range distances. However, if the spin singlet is sufficiently close togeher, while inserted into a magnetic field one might expect (depending on their closeness) that the induced magnetic effect of each particle will be equal and opposite and result in them being repelled by each other, analogous to the repulsion between currents flowing in oppposite directions in two parallel wires. In contrast, if the spin orbital is composed of two electrons in the parallel spin state, one might expect that when they are immersed in a magnetic field the induced magnetism will cause them to attract each other if they lie in the same plane perpendicular to the magnetic field. This is analogous to currents flowing in the same direction in two parallel wires [34]. Obviously many other factors are involved including the orientations of all the different ISC states within the molecule, the electric repulsion among the electrons, temperature and pressure. In fact, the $|\psi\rangle_2$ state is invariant under the action of SL(2,C) regardless of orientation, while the parallel state is rotationally invariant over a plane, which gives a mathematical justification

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based on rotational invariance for the observation that "there is a nodal plane along the internuclear axis for all pi molecular orbitals"[35]. For this reason when the σ^* orbitals (associated with the $|\psi\rangle_1$ state) are side-by-side the paramagnetic effect should be enhanced and attractive.

The above examples, hopefully, serve as a justification for replacing what is usually referred to in the literature as *unpaired electrons with parallel spin*, with the ISC state $|\psi\rangle_1$, which can be associated with a rotationally invariant pair of electrons in the same spin state. Morever, the rotational invariance also enables us to predict the existence of spin-singlet states in the same orbitals (in the traditional sense of the word) and in different orbitals (again in the traditional sense of the word). The group theory puts no restrictions on the other quantum numbers. Consequently, two electrons can share the same quantum numbers (except for spin) meaning that they are in the same orbital or they can have different quantum numbers (meaning they are in different orbitals) but form a spin-singlet state. Indeed, this is what has been observed in “the three forms of molecular oxygen” [24]. To repeat, the group theory indicates the types of rotational invariance associated with chemical bonding. However, it imposes no other restrictions. In remains for the chemists to integrate this with the other laws of chemistry based on Hund’s rules and the Pauli exclusion principle.

3.2. Fermi-Dirac Statistics and Entanglement

The Pauli exclusion principle is considered a key instrument in understanding chemical bonding and is often considered as a law in its own right. As it turns out, it can be derived by combining the notion of rotational invariance and indistinguishability. There are two approaches: The first is to show that the existence of n indistinguishable ISC states $|\psi\rangle_2$ is equivalent to the Pauli exclusion principle. A proof can be found in [10]. Indeed, as the indistinguishability condition is relaxed different types of parastatistics emerge including identifying superconducting states with standing waves of ISC pairs. One class of superconductors can be associated with standing waves of multiple singlet states $|\psi\rangle_2$ and another with the rotationally invariant paired states $|\psi\rangle_1$. From this perspective superconducting Cooper pairs are a special case [11].

However, it might be asked if there are multivariate systems of higher dimensions composed of indistinguishable particles that are rotationally invariant. As it turns out, an indistinguisable quantum state composed of ISC pairs obeys the Fermi-Dirac statistics. More precisely, it can be shown that a necessary and sufficient condition for Fermi-Dirac statistics is that the state be invariant under the action of $SL(n, \mathcal{C})$. Indeed, the Fermi-Dirac state is (uniquely) invariant under the action of the $SL(n, C)$ group, which a fortiori means that it is invariant for all subgroups of $SL(n, C)$, including the rotation group. The only exception is in the case of two-dimensional subspaces $C^2 \subset C^n$, where there are two rotationally invariant states and not one. As already noted in the previous section, this arises from the mathematical properties associated with Clifford algebras. In general if $\mathbf{u}$ and $\mathbf{v}$ are two vectors in C^n then we can define a Clifford product by

$$\mathbf{uv} = \mathbf{u.v} + \mathbf{u} \wedge \mathbf{v}$$

The first term corresponds to an inner product which can be defined for any pair of vectors and such a product is always rotationally invariant. However, there is no inner prodect for three vectors $\mathbf{u}$, $\mathbf{v}$, $\mathbf{w}$, meaning that $\mathbf{u.v.w}$ is not defined. In contrast, outer (wedge) products are defined over n-dimensions and correspond geometrically to volume (area in 2-dim), which is preserved under rotations. This leads to the invariance of the Fermi-dirac state under SL(n,C) as proven in the following theorem[36]:

Theorem 2. *Let* $V = W_1 \otimes \cdots \otimes W_n$*, be a vector space, with each* W_i *an* n*-dimensional subspace (up to isomorphism),* $T = T_1 \otimes \cdots \otimes T_n$*, with* $T_i = T_j$ *for each* i *and* j *and* T_i *a linear operator on* W_i*. If*

$$\begin{aligned} v &\equiv w_1 \wedge w_2 \wedge \cdots \wedge w_n \\ &= \begin{pmatrix} w_{11} \\ \vdots \\ w_{n1} \end{pmatrix} \wedge \begin{pmatrix} w_{12} \\ \vdots \\ w_{n2} \end{pmatrix} \wedge \cdots \wedge \begin{pmatrix} w_{1n} \\ \vdots \\ w_{nn} \end{pmatrix} \end{aligned}$$

then for $v \neq 0$

$$Tv = v \iff T \in \bigotimes_{1}^{n} SL(n, \mathcal{C}).$$

This means Fermi-Dirac statistics is invariant under the action of $SL(n, \mathcal{C})$.

Proof of Theorem 2. For each W_i, we can associate an orthonormal basis $\{\mathbf{e}_1, \mathbf{e}_2 \ldots \mathbf{e}_n\}$. Therefore

$$\begin{aligned} v &= \begin{pmatrix} w_{11} \\ \vdots \\ w_{n1} \end{pmatrix} \wedge \begin{pmatrix} w_{12} \\ \vdots \\ w_{n2} \end{pmatrix} \wedge \cdots \wedge \begin{pmatrix} w_{n1} \\ \vdots \\ w_{nn} \end{pmatrix} \\ &= |v| \mathbf{e}_1 \wedge \mathbf{e}_2 \wedge \cdots \wedge \mathbf{e}_n \end{aligned}$$

where

$$|v| = \begin{vmatrix} w_{11} & w_{12} & \cdots & w_{1n} \\ w_{21} & w_{22} & \cdots & w_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ w_{n1} & v_{n2} & \cdots & w_{nn} \end{vmatrix}.$$

It follows from the linearity of T that

$$\begin{aligned} Tv &= |v| T_1 \mathbf{e}_1 \wedge T_2 \mathbf{e}_2 \wedge \cdots \wedge T_n \mathbf{e}_n \\ &= |v| \begin{pmatrix} t_{11} \\ \vdots \\ t_{n1} \end{pmatrix} \wedge \begin{pmatrix} t_{12} \\ \vdots \\ t_{n2} \end{pmatrix} \wedge \cdots \wedge \begin{pmatrix} t_{n1} \\ \vdots \\ t_{nn} \end{pmatrix} \\ &= |v||T_1| \mathbf{e}_1 \wedge \mathbf{e}_2 \wedge \cdots \wedge \mathbf{e}_n, \qquad T_1 = T_2 = \cdots = T_n \end{aligned}$$

But $v \neq 0$ implies $|v| \neq 0$ and therefore

$$Tv = v \Rightarrow |T_1| = 1 \text{ and } T_1 \in SL(n, \mathcal{C}) .$$

Conversely,

$$T_1 \in SL(n, \mathcal{C}) \Rightarrow Tv = v .$$

The theorem has been proven. Moreover, v is unique as demonstrated in [36]. □

The observant reader might be wondering how this relates to Pauli's original paper on the spin-statistics theorem[6]. Pauli's proof as a point of departure assumes the validity of the principle of microcausality. Translated into operator language this means that conjugate operators must commute beyond the light cone to preserve independence. However, in the case of ISC states this breaks down. Operators and in particular Pauli's spin operators, indexed by different spacetime coordinates, are completely interchangeable because of the entanglement. This means that the associated Clifford (Dirac) algebra may or may not commute beyond the light cone. In the case of ISC states the algebraic characteristics of the Pauli spin matrices applied to one particle of the bivariate state, instanteously allows us to predict the spin characteristics of the second particle, which means that the information can be determined beyond the light cone.

Specifically, consider a two particle (bivariate) system $|\psi(\lambda_1)\rangle \otimes |\psi(\lambda_2)\rangle \in \mathcal{S}_1 \otimes \mathcal{S}_2$ where $\mathcal{S}_1 = \mathcal{L}^2(\mathcal{R}^3) \otimes H_1$ and $\mathcal{S}_2 = \mathcal{L}^2(\mathcal{R}^3) \otimes H_2$ respectively [37]. Note that each ket $|\psi(\lambda)\rangle \in \mathcal{S}$ can be written as $|\psi(q_1)\rangle \otimes s$, where s is a spinor. Also, let $\vec{S}_1 = (S_i(q_1), S_j(q_1), S_k(q_1))$ and $\vec{S}_2 = (S_i(q_2), S_j(q_2), S_k(q_2))$ be spin operators defined on the Hilbert spaces H_1 and H_2 respectively. If both particles are considered statistically independent of each other then individual measurements on each one are separated by a spacelike distance and will be represented respectively by operators of the form $S_i(q_1) \otimes I_2$ and $I_1 \otimes S_j(q_2)$. It follows, trivially, that $[S_i(q_1) \otimes I_2, I_1 \otimes S_j(q_2)] = 0$, which means all measurements will commute beyond the light cone, as for example that in the case of the triplet state given by equation (6).

In contrast, the singlet state is ISC. In this case, it would be inappropriate to apply the operators for independent states. Instead, we let $|\psi(\lambda_1, \lambda_2\rangle \in \mathcal{S}_1 \otimes \mathcal{S}_2$ represent the spin-singlet state of two particles. Note that the perfect correlations between them allows us to put $H_1 = H_2 = H$ and to identify $\vec{S}_1$ and $\vec{S}_2$ as follows: Let $s_1(\theta)$ and $s_2(\theta)$ represent the spin states for particles 1 and 2 respectively then for an arbitrary angle θ there exists a unit vector $\vec{n}(\theta)$ such that $\vec{S}_1.\vec{n}(\theta)(s_1(\theta)) = \pm s_1(\theta)$ if and only if $\vec{S}_2.\vec{n}(\theta)(s_2(\theta)) = \mp s_2(\theta)$. This relationship allows us to identify $s_2(\theta)$ with the orthogonal complement $s_1^-(\theta)$ of $s_1(\theta)$ and to put $\vec{S}_1 = \vec{S}_2$.

This identification means that $\vec{S}_1.\vec{n}(\theta) = \vec{S}_2.\vec{n}(\theta)$ (note the same θ) and therefore $[\vec{S}_1.\vec{n}(\theta), \vec{S}_2.\vec{n}(\theta)] = 0$. However, because of the nature of entanglement we also free to consider $\vec{S}_1.\vec{n}(\theta_1)$ and $\vec{S}_2.\vec{n}(\theta_2)$ where $\theta_1 \neq \theta_2$ and in this case $[\vec{S}_1.\vec{n}(\theta_1), \vec{S}_2.\vec{n}(\theta_2)] \neq 0$. In fact, $[S_i, S_j] = in\epsilon_{ijk}S_k$.

Simply put, microcausality does not apply to entangled states. Entanglement permits both zero and non-zero commutators. It is an example, as noted in the introduction, of one measurement yielding two pieces of information. Rather than asking if events are spacelike or timelike, we should first ask if they are correlated or uncorrelated and based on that answer then consider whether spacelike or timelike has any meaning.

Microcauslaity presupposes quantum locality. Entanglement as demonstrated by Bell's theorem [14] and verified experimentally by Aspect et al. [38], is a non-local phenomenon and consequently the principle of microcausality is violated by ISC states, where one measurement instantaneously yields two pieces of information. Pauli makes no reference to entanglement is his paper. It was not an issue in his day. However, he does note that if the principle of microcausality fails then the statistical distinction between integral and half-integral spin also breaks down ([6], p721). The above theorem clearly implies that a superposition of n indistinguisable ISC states is equivalent to the Fermi-Dirac statistic, and that the Bose-Einstain statistic follows as a consequence of breaking the ISC condition. It is the ISC properties of spin or the lack thereof that determine the characteristics of quantum statistics. Spin value plays no role.

3.3. Group Classification of Entangled States

With the above theorems now in place, we are in a position to further classify engangled states using group theory. We distinguish between states comprised of singlet states but with different degrees of reducability with respect to $SL(n, C)$ group. Specifically,

$$c_1 SL(n_1, C) \oplus \cdots \oplus c_n SL(n, C) \iff |\psi\rangle = c_1|\psi\rangle_1 \oplus \cdots \oplus c_m|\psi\rangle_m$$

where it is understood that $SL(n_i, C)|\psi\rangle_i = |\psi\rangle_i$ and c_i is the multiplicity. In other words, for any entangled states constructed from the Bell states (which are rotationally invariant) we can classify n-dimensional Bell entangled states according to the degree of indistinguisability that is permitted. If a state is invariant under the group $SL(n, C)$ then it will also be invariant under the group S_n, this follows from the fact that the a Fermi-Dirac state is always invariant under the permutation group. For example, consider a set of 6 electrons. These could be the 6 electrons of a carbon atom, or the 5 electrons of boron and 1 of hydrogen, or the 4 electrons of beryllium and 2 of helium, or the 3 electrons

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in two different lithium atoms. Each of these cases can be respectively classified as invariant under the action of the groups

$$Sl(6,C),\ SL(5,C)\oplus I,\ SL(4,C)\oplus SL(2,C),\ SL(3,C)\oplus SL(3,C),$$

which also serve as a specification of the degree of entanglement for each component. Note that the last case has multiplicity 2.

In the case of the molecules Li_2 with the orbital structure $2\sigma_{1s}, \sigma_{2s}$, the group classification would be given by $SL(2,C)\otimes SL(2,C)\otimes SL(2,C)$. where the two independent lithium atoms (spin triplet state) would have a group structure $SL(3,C)\otimes SL(3,C)$. In the case of the boron molecule B_2 the bond structure is given by $2\sigma_{1s}, 2\sigma_{2s}, \sigma^*_{2p}$ which can be identified with the group structure $SL(2,C)\otimes SL(2,C)\otimes SL(2,C)\otimes SL(2,C)\otimes SO(2,C)$, where the $SO(2,C)$ defines a two dimensional rotational group.

3.4. Perfect Correlations and ISC States

The preceding sections have focused on bivariate entanglement composed of ISC or rotationally invariant states. As we have noted, in the case of a bivariate system there are essentially only two entangled states both of which are rotationally invariant and ISC. They can be combined to form a Clifford algebra which again maintains the rotationally invariant property. Nevertheless, it is important to point out that although ISC states are both rotationally invariant and perfectly correlated, they are two different concepts. ISC states in general refer to bivariate systems, while perfectly correlated states refer to multivariate systems involving three or more tensor products of single states. They are defined by Greenberger, Horne, Shimony and Zeilinger [7] in their paper “Bell’s theorem without inequalities” and are usually referred to as GHZ states. To further explore the meaning of entanglement within the context of multivariate states, we will refer to their article (herein referred to by the acronym GHSZ). Another important study in this regard can be found in [39]. It might be worth noting that in terms of entanglement in general, the Bell states serve as seed states for "entangled entanglement" and can be used to construct GHZ states through a process of iteration [40].

According to GHSZ, an entangled state is such that “it cannot be written in any way as a product of single-particle states"(p1132). This means that an entangled cannot be written in the form

$$|\psi\rangle = |\psi_1\rangle|\psi_2\rangle\dots|\psi_n\rangle$$

This is is in agreement with Definition 1 of this article.

In general, if we are in the space $\mathcal{C}^3$, defined over the complex numbers, a threefold entangled state can be written as a linear combination of $3^3 = 27$ (complex) terms in the form

$$\sum \alpha_{ijk}|\psi_i\rangle|\psi_j\rangle|\psi_k\rangle$$

where each $i,\ j,\ k,\in \{1,2,3\}$. From a mathematical point of view, depending on the values of α_{ijk} there are an infinite number of three particle entangled states. In practise, we focus on certain specific states of interest to physics. For example, if $i\neq j\neq k$ then it will reduce to a state of only six terms, and if we further require that it be composed of indistinguishable terms then it will reduce to a Fermi-Dirac or Bose-Einstein state. It remains an open question whether every possible mathematically entangled state can be physically realized.

If $i,\ j,\ k$ are restricted to only two values (qubits) then the threefold entangled state can be written as a linear combination of $2^3 = 8$ terms, as is the case with the GHZ state defined by equation (G1) of GHSZ. It is given by

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$$\begin{array}{ll} \frac{1}{4}[(1-ie^{i(\phi_1+\phi_2+\phi_3)}|d\rangle_1)|e\rangle_2|f\rangle_3 & +(i-e^{i(\phi_1+\phi_2+\phi_3)}|d\rangle_1)|e\rangle_2|f'\rangle_3 \\ +(i-e^{i(\phi_1+\phi_2+\phi_3)}|d\rangle_1)|e'\rangle_2|f\rangle_3 & +(-1+ie^{i(\phi_1+\phi_2+\phi_3)}|d\rangle_1)|e'\rangle_2|f'\rangle_3 \\ +(i-e^{i(\phi_1+\phi_2+\phi_3)}|d'\rangle_1)|e\rangle_2|f\rangle_3 & +(-1+ie^{i(\phi_1+\phi_2+\phi_3)}|d'\rangle_1)|e\rangle_2|f'\rangle_3 \\ +(-1+ie^{i(\phi_1+\phi_2+\phi_3)}|d'\rangle_1)|e'\rangle_2|f\rangle_3 & +(-i+e^{i(\phi_1+\phi_2+\phi_3)}|d'\rangle_1)|e'\rangle_2|f'\rangle_3] \end{array}$$

These states are particularly interesting in that they represent the evolution of the GHZ state given by

$$|\psi\rangle = \frac{1}{\sqrt{2}}[|a\rangle_1|b\rangle_2|c\rangle_3 + |a'\rangle_1|b'\rangle_2|c'\rangle_3 \tag{30}$$

where $|a\rangle_1 \rightarrow \frac{1}{\sqrt{2}}[|d\rangle_1 + i|d'\rangle_1]$ and $|a'\rangle_1 \rightarrow \frac{1}{\sqrt{2}}[|d'\rangle_1 + i|d\rangle_1]$. It should be apparent from this transformation that $|\psi\rangle$ is not rotationally invariant even when $\phi_1+\phi_2+\phi_3 = 0$, whereas when projected into a two dimensional state with $\phi_1+\phi_2 = n\pi$ it is rotationally invariant under (R, R^T), where R is a two-dimensional rotation matrix.

The general GHZ state for three particles presupposes that if we measure (observe) the states $|a\rangle$ and $|b\rangle$ then $|c\rangle$ would be determined by the other two. However, in the case of an ISC state only **one** measurement would determine the other two. In other words, if we were to observe $|a\rangle$ then both $|b\rangle$ and $|c\rangle$ would be determined in the direction of measurement. However, as pointed out in Theorem 1 (Section 4) ISC states can only occur in pairs. The authors of GHSZ paper, although they do not speak of ISC states per se, are aware that the Bell states differ from higher dimensional states. In their Appendix A, they clearly point out and prove the rotational invariance of the singlet state (equation (A3)), while in Appendix B (although they do not develop it further) they imply that there is a difference between ISC states (my terminology) and "a rotationally invariant **mixture** of product states, which will not yield correlations as strong as [the singlet] $|\psi\rangle$ does." They then preceed to give an example.

Finally we note that in terms of GHZ states, rotational invariance is only applied to the two particle singlet state (paired qubits). There is no reference to other GHZ states being rotationally invariant, instead they refer to polarized states. Apart from the bivariate state, the other GSZ states are not rotationally invariant, although they obey other group properties. For example, the GHZ states given by equation (30) and its evolved states are not invariant under rotations but they are invariant under the action of the finite group of order eight $\mathcal{Z}_2 \times \mathcal{Z}_2 \times \mathcal{Z}_2$. In the case of entangled states that are NOT generated by the Bell states then the rotational invariance is lost and each case should be classified according to its degree of polarization specified by the permutation group.Similarly, the perfectly correlated state

$$\frac{1}{\sqrt{2}}[|+\rangle_1|+\rangle_2|-\rangle_3|-\rangle_4 - |-\rangle_1|-\rangle_2|+\rangle_3|+\rangle_4]$$

is invariant (up to sign) under the group $\mathcal{Z}_2 \otimes \mathcal{Z}_2 \otimes \mathcal{Z}_2 \otimes \mathcal{Z}_2$.

4. Discussion

The article has pointed out that the rotational properties of quantum spin entanglement underlies a coupling principle which states that isotropically spin-correlated particles must occur in pairs. In turn, this pairing phenomenon can be used to derive and give a more intuitive understanding of the Pauli exclusion principle, serve as a unifying principle to explain conventional and unconventional superconductors, as well as bonding and anti-bonding interactions in chemistry. In other words, if the pairing process is taken as a point of departure, then all of these phenomena share something in common, which as the article has pointed out, is a result of the rotational invariance of entangled states. Even the Fermi-Dirac statistic can be interpreted as a consequence of combing indistinguishablity with particle pairing.

5. Conclusions

The article has discussed how group theory can add to our understanding of entanglement and molecular bonding. It has been pointed out that different types of entanglement can be associated with a group structure that leaves invariant the entangled state, and this structure can be associated with the degree of indistinguisability within the particle configuration. Conversely, if we know the group configuration of the particles , we can also specify the degree of indistinguisability among them. Group theory enables us to identify symmetries within the entangled state, although it does not distinguish which ISC state is more probable. In the bivariate case in particular, the building blocks of entangled states are the two ISC states, which can be combined to form a Clifford algebra, with each component being respectively invariant under the action of the rotation group and the $SL(2, \mathcal{C})$ group. Multivariate entangled states defined over $\mathcal{H}_1 \otimes \ldots \mathcal{H}_n$ also exist for $n \geq 3$ but with the exception of the Fermi-Dirac state, they are not rotationally invariant and are best classified by some type of finite group. Indeed, apart from the two ISC states all other entangled states are polarized states with the entanglement applying to specific directions. The one exception is the Fermi-Dirac statistic which is $SL(n, \mathcal{C})$ invariant and is composed of n ISC indistinguishable states.

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References

1. C. Brukner, M. Zukowski, A. Zeilinger. “The Essence of Entanglement.” *Fundamental Theories of Physics*,**2001**. doi: $10.1007/978-3-030-77367-0_6$
2. M. Land. “Covariant Representation of Spin and Entaglement – A Review and Reformulation.” *Symmetry***2024**, 16(11), p. 1465. doi: 10.3390/sym16111465
3. E. Adlam. “How are Entanglement Entropies Related to Entropy Bounds.’ *Phil. of Physics 2(1)*,**2024**, p. 9. 10.31389/pop.109
4. J. von Neumann. *Mathematical Foundations of Quantum Mechanics.* 1st ed; Princeton U, Princeton, USA,1996 (12th printing).
5. R. Tolman. *The Principles of Statistical Mechanics.* Dover Publ., NY (1979), p. 328.
6. W. Pauli. “The Connection Between Spin and Statistics." *Phys. Rev***1940**, 716-722. doi: 10.1103/PhysRev.58.716
7. D. Greenberger, M. Horne, A. Shimony, A. Zeilinger. “Bell’s theorem without inequalities.” *Am. J. Phys. 58 (12)*,**1990** pp. 1131-1143. doi:10.1119/1.16243
8. C. Bennett, D. DiVincenzo, J. Smolin, W. Wooters. “Mixed State entanglement and Quantum Error Correction.” *Phys. Rev. A* **54**, *3825, 1996.* doi:10.1103/PhysRevA.54.3824
9. P. O’Hara. “Entanglement – A Higher Order Symmmetry.” *Phys. Sci. Forum***2023** 7(1) doi:10.3390/ECU2023-14011
10. P. O’Hara. “Rotational Invariance and the Spin-Statistics Theorem.” *Found of Phys.* Vol. 33, No. 9, pp 1349-1368. doi:10.123/A:1025697412645
11. P. O’Hara. “Spin Entanglement - A Unifying Principle for Superconductors and Molecular Bonding.” *Recent Progress in Materials. Special edition: Quantum Mechanics in Solid State Systems***2024**. doi:10.21926/rpm.2402012.
12. A. Einstein, B. Podolsky ,N. Rosen. “Can Quantum-Mechanical Description of Physical Reality Be Considered Complete?" *Phys. Rev.***1935**, *47*, 777-780. doi: 10.1103/PhysRev.47.777
13. E. Wigner. “On hidden variables and quantum mechanical probabilities.” *Am. J. Phys.***1970**, *38*, 1005. doi:10.1119/1.1976526
14. J. Bell. “On The Einstein Podolsky Rosen Paradox." *Physics***1964** *1*, 195-200. doi: 10.1103/PhysicsPhysiqueFizika.1.195
15. K. Ueda et al. “Dominant nonlocal superconducting proximity effect due to electron-electron interaction in a ballistic double nanowire.” *Science Advances***2019**,*5(10)*. doi: 10.1126/sciadv.aaw2194
16. J. Bardeen. “Electron-Phonon Interactions and Superconductivity.” *In H.Haken and M. Wagner (ed.): Cooperative Phenomena*, Springer, 1973 p. 67. doi: 10.1007/978-3-642-86003-4-6
17. I. Bozovic, J. Levy. “Pre-formed Cooper pairs in copper oxides and $LaAIO_3 - SrTiO_3$ heterostructures.” *In Nature Physics* 16, 712-717, (2020). doi: 10.1038s4157-020-0915-8

18. P. Chaovsky. "Bose-Einstein Condensation of Rubidium Atoms." *In JETP Letters*, 2012, Vol. 95, No. 3, pp 132-136. doi:10.1134/S0021364012030046
19. E. Donley, N. Claussen, S. Thompson, C. Wieman. "Atom-molecule coherence in a Bose-Einstein condensate." *In Nature*, 417, 529-533 (2002). doi:10.1038/417529a
20. J. Georgescu. "25 years of BEC.' *In Nature Reviews Physics*,**2** 396(2020) doi:10.1038/s42254-020-0211-7
21. A. Gezerlis. "Strongly paired fermions: Cold atoms and neutron matter." *In Phys. Rev C*, [77] (3) 032801. doi: 10.1103/PhysRevC.77.032801
22. H. Huang, S. Karan, C. Padurariu et al. "Universal scaling of tunable Yu-Shiba-Rusinov states across the quantum phase transition." *In Commun Phys* 6, 214 (2023). doi:10.1038/s42005-023-01332-8
23. A. Kovàcs, G. Vassallo. "High-temperature superconductivity is the catalyzed Bose-Einstein condensation of electrons." *In Amazon*, pp. 17-19 (2023). doi:ISBN:978-9526531403
24. M. Laing. "The Three Forms of Molecular Oxygen." *In Journal of Chemical Education*, **1992**, p.340.
25. R. Madden, K. Codling. "New Autoionizing Atomic Energy Levels in He, Ne, and Ar." *Physical Review Letters*, Volume 10, 516 (1963). doi:10.1103/PhysRevLett.10.516
26. NIST. "Strontium Unlocks the Quantum Secrets of Superconductivity." *In SciTech Daily*, March 11 2024.
27. M. Piestrup, H. Puthoff, P. Ebert. "Enhanced Correlated-Charge Field Emission" (1998). doi: 10.21236/ada337858
28. T. Orlando, K. Delin. "Foundations of Applied Superconductivity." *In Prentice Hall*, 1991. $doi : 10.1007/978 - 1 - 4615 - 5075 - 4_7$
29. S. Ran. "Unboxing a New Spin-Triplet Superconductor." *In NIST*, www.nist.gov/blogs/taking-measure/unboxing-new-spin-triplet-superconductor, Nov 19., 2019.
30. S. Ran et al. "Nearly ferromagnetic spin-triplet superconductivity." *In Science*, 2019. doi:10.1126/science.aav8645
31. S. Karan, H. Huang, C. Padurariu. et al. "Superconducting quantum interference at the atomic scale." *In Nat. Phys.* 18, 893–898 (2022). doi:10.1038/s41567-022-01644-6
32. D. Young, A. Chu, E. Song et al. "Observing dynamical phases of BCS superconductors in a cavity QED simulator" *In Nature*, Jan. 24, 2024 doi:10.1038/s41586-023-06911-x
33. D. Hestenes, G. Sobczyk. *Clifford Algebra to Geometric Calculus.* Springer, 1984. 1st ed.
34. P. Lorraine, D. Carson *Electromagnetic Fields And Waves.* Freeman Co., 2nd edition, pp. 297-298.
35. K. Witten, K. Gailey, R. Davis. *General Chemistry.* Saunders College Publ. 4th edition
36. P. O'Hara. "A generalized spin-statistics theorem." *In J. Phys. Conf. Ser.*, 2017, 845, 012030. $doi : 10.1088/1742 - 6596/845/1/012030$
37. P. O'Hara. ''Entanglement, Microcausality and Godel's Theorem." *In 2023 J. Phys.: Conf. Ser.*, 2023 2482 012013 DOI 10.1088/1742-6596/2482/1/012013
38. A.Aspect, J. Dalibard, G. Roger. "Experimental Test of Bell's Inequalities Using Time Varying Analyzers" *Phy. Rev. Letts.***1982**, *49*, 1804-1807.
39. D. Greenberger, M. Horne, A. Zeilinger. "Going Beyond Bell's Theorem." *Bell's Theorem, Quantum Theory, and Conceptions of the Universe; Kafatos(ed), Menos(ed); Springer: Heidelberg, Germany* pp. 69-72.
40. G. Uchida, R. Berthmann, B. Hiesmayr "Entangled Entanglement: A construction procedure" *In Phys. Lett. A*, Volume 379 (42), 2015, pp. 2698-2703. doi:10.1016/j.physleta.2015.07.045.