Excluded states in entangled systems: technical and conceptual aspects

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Abstract

The impossibility of ascribing definite states to the constituents of an entangled system restricts the scope of Pauli’s principle in this context. We analyze the conceptual and physical aspects of the problem by studying the actual scope of the principle and the possibility of extending the concept of exclusion in correlated systems. When the entanglement is weak, as in the archetypical case of the Helium atom, the principle can be applied in an approximated way. The concept of non-complete set of properties plays a crucial role in the argument, which also clarifies the physical meaning of the atomic quantum numbers; they are a multi-particle property, not an one-electron one. In contrast, for strong entanglement the excluded states are independent of the principle. We describe some of these states, many times determined by symmetries of the multi-fermion state.

1 Introduction

Pauli’s exclusion principle [1] is a fundamental tool to describe the behavior of identical fermions. It states that two identical fermions cannot be in the same physical state. Implicit to this formulation is the assumption that individual fermions are in definite states. This is a natural assumption for product states, but becomes problematic for entangled ones. When a multi-particle system is in an entangled state there is a state of the complete system but there are not individual states of the particles composing it. This well-known fact can also be formulated in terms of properties of the particles: when the system is entangled one cannot attribute complete sets of properties to the constituents [2, 3, 4, 5]. If the constituents have not individual states the exclusion conditions cannot be used in the standard way.

Technical and conceptual questions immediately arise from the above considerations. We shall discuss both simultaneously in an interconnected way. It is well-known that the principle has been successfully applied to explain the
structure of some entangled systems as atoms. We shall show, in the case of
the Helium atom, that this fact can be explained because a weak entanglement
approximation works well. Within the weak entanglement approximation it is
possible, in some cases, to ascribe individual states to the two electrons. Some
of them are excluded by Pauli’s principle, explaining the energy levels structure
of the atom. In addition, our approach clarifies a subtle aspects of the problem.
In the weak entanglement regime it is possible to define non-complete sets
of spatial and spin properties. Although these partial properties cannot define
one-electron states, they can be used to justify the definition of quantum num-
bers in the system. However, contrarily to a naive expectation, these numbers
are related to the full two-electron state, not individually to each electron. The
quantum numbers are multi-particle properties.

After clarifying the above point another question appears in a natural way:
are there excluded states when the weak entanglement approximation cannot
be invoked? In such a regime of strong entanglement Pauli’s principle does not
make sense. We answer this question in the affirmative. One can define ex-
cluded states in the same mathematical way associated with Pauli-type ones:
for some conditions (equality of states in the standard case) the state becomes
undefined. We identify some of these generalized excluded states, whose exclu-
sion conditions are mainly related to the symmetries of the multi-fermion state
previous to antisymmetrization.

2 States and properties in entangled systems

Pauli’s principle is a physical statement based on the states of the constituents of
the system. When the system is entangled the definition of these states becomes
a subtle subject, specially when the components are identical particles. In this
section we review the main aspects of the problem.

Let us begin with the simpler case of distinguishable (non-identical) par-
ticles. By the sake of simplicity we restrict our considerations to two-par-
ticle systems. The extension to the general case is straightforward. We con-
sider a couple of particles with only one degree of freedom, the spatial one (for instance, spin-0
particles). If we label \( A \) and \( B \) the two types of particles a typical example of
entangled state is

\[
|\Psi> = \frac{1}{\sqrt{2}} (|L>A |R>B - |R>A |L>B) \tag{1}
\]

with \( L \) and \( R \) denoting two non-overlapping, and consequently orthogonal, spa-
tial locations. From \( \Psi \) we cannot ascribe one-particle states to \( A \) and \( B \). We
cannot say anything about the state of \( A \) without reference to the state of \( B \),
and vice versa. The same conclusion can be reached via the reduced density
matrix of \( A \), which is obtained by tracing out over \( B \) the two-particle density
matrix \( |\Psi><\Psi|: \rho_A = (<L<<L|+|R<<R|)/2 \). This is an improper mixture
that cannot be associated with a pure state. There are not one-particle pure states in entangled systems.

An alternative, and very powerful from the conceptual point of view, way to analyze the subject was pioneered by Ghirardi et al. [2, 3, 4]. It is based on the consideration of properties instead of states. In the case of systems in product states these properties can be easily ascribed. For instance, in the state $|L >_A |R >_B$ we can say that the particle $A \ (B)$ has the physical property of being located at $L \ (R)$. A position measurement would corroborate this assignment. In contrast, for the entangled state $\Psi$ the localization of the particles is undetermined; they do not have the physical property of being located at specific regions of space. This approach is in the spirit of the Einstein-Podolsky-Rosen argument, because measurements carried out on the observable associated with the assigned property will give with certainty that value.

The above conclusions, the absence of one-particle states and properties for entangled systems, cannot be directly translated to the case of identical particles. In this case the notion of entanglement is much more subtle and there is no complete agreement on its correct characterization yet. The reason for these difficulties lies on the introduction of labels in the symmetrization process that are not physical degrees of freedom. For instance, a state of the type (1) specialized to identical particle reads $|\Psi_{ide} >= (|L >_1 |R >_2 - |R >_1 |L >_2 )/\sqrt{2}$, where the labels $A$ and $B$ of distinguishable particles have been replaced by 1 and 2, indicating that now we are dealing with identical particles. Although apparently the states $\Psi$ and $\Psi_{ide}$ share the same type of non-factorizability, there are actually fundamental differences between them. The states like $\Psi_{ide}$ that represent the (anti)symmetrization of a product state (in our example $|L >_1 |R >_2$) are not really entangled. It is easy to demonstrate that they are not a resource of non-classical correlations, the trademark of entangled states. This point has been discussed in detail in [4, 6] for violations of Bell’s inequalities and in [6] for quantum information processing. Thus, as signaled in [6], the apparent entanglement of states like $\Psi_{ide}$, suggested by their non-factorizability, is only an artifact of a formalism with surplus structure. Nevertheless, it must be stressed that this surplus character only refers to entanglement. There are other physical processes, like interference, that are sensitive to the (anti)symmetrized form of the states of identical particles (see, for instance, [6, 7]).

All these and other considerations led to the definition of entanglement for systems of identical particles proposed in [2]: a system of identical particles is entangled when it is impossible to ascribe a complete set of properties to each constituent. Note that the set of properties must be complete, that is, we must have a property for each degree of freedom of the particle. This is the definition of entanglement of identical particles we shall follow in the paper. Now, we are in position to give an answer to the question of the existence of individual states for entangled identical particles. As the physical properties of the constituents are mathematically represented by one-particle states this definition of entanglement automatically precludes the existence of individual
states.

If there are not states of the particles we will not be able of individuating the 
constituents of the system. There have been many discussions in the literature 
about how individuating quantum particles [8]. In classical physics we are able 
to individuate even identical particles (with all their intrinsic properties equal) 
via their positions. Unfortunately, this approach fails in quantum theory, where 
localization is not so sharp. The only possibility of individuating identical par-
ticles in the quantum realm is via the relevant observables and pure states. The 
operators associated with the observable and the pure states provide a com-
plete set of properties [8]. When the system is entangled these states simply do 
do not exist, precluding any attempt of distinguishing the constituents by physical 
means. The labels associated with the (anti)symmetrization procedure are only 
mathematical artifacts deserved of any connection with physical properties.

The above discussion clearly indicates that we must rethink the subject. The 
theory of excluded multi-fermion states, usually based on one-fermion states and 
Pauli’s principle, should be formulated in a different way. As we shall discuss 
at length in the rest of the paper such a formulation can be done based on 
two properties of the system. The first one is the possibility of defining partial 
properties of the constituents. The second one refers to exclusion conditions 
based on properties of the multi-fermion state.

3 Pauli’s principle in the Helium atom

The aim of this section is to justify the existence of quantum numbers and the 
application of Pauli’s principle in some entangled atomic systems. Being these 
systems entangled, without individual states of the electrons, the validity of 
these two properties is not obvious at all. The analysis will show the importance 
of the concept of partial sets of properties in the problem.

We restrict our considerations to the simplest case, the Helium atom. The 
generalization to other atoms is simple. As it is well-known, the states describing 
the two electrons in the Helium atom are the product of the spatial and spin 
states, and they can be written in three different forms

$$|\Psi_\pm > = N_\pm (\psi(x,y) \pm \psi(y,x))(|s >_1 |s' >_2 \mp |s' >_1 |s >_2)$$ (2)

and

$$|\Psi_\ast > = N_\ast (\psi(x,y) - \psi(y,x))|s >_1 |s >_2$$ (3)

with

$$N_\pm = (4(1 \pm Re(\langle \psi(x,y) |\psi(y,x) >))(1 \mp |\langle s |s' > |^2))^{-1/2}$$ (4)

and

$$N_\ast = (2(1 - Re(\langle \psi(x,y) |\psi(y,x) >))^{-1/2}$$ (5)
the normalization factors (provided that \( \psi \) is normalized). For \( \Psi_+ \) we symmetrize the spatial part and antisymmetrize the spin one (and vice versa for \( \Psi_- \) and \( \Psi_+ \)). In all the cases the complete state is antisymmetrized. At variance with textbook presentations of the problem the spatial wavefunction has not a product form, reflecting the mutual interaction of the electrons. In the atomic physics jargon, \( \Psi_- \) and \( \Psi_+ \) are ortho-Helium type states and \( \Psi_+ \) is a para-Helium type one.

Note that we have used the antisymmetrization principle in its standard form. The arguments supporting this principle are independent of the factorizable or non-factorizable nature of the state. Then they are valid for both entangled and product states.

The non-factorizable states of identical particles have two types of contributions to the non-separability, those due to antisymmetrization and to entanglement. It is necessary to distinguish between them in order to correctly identify the true entanglement. According to the criterion in [2] a two-fermion state is non-entangled if and only if it is obtained by antisymmetrizing a factorized state. Applying the criterion to the previous examples we have that the states \( \Psi_\pm \) are entangled. On the other hand, \( \Psi_\ast \) corresponds to the antisymmetrization of the state \( \psi(x,y)\ket{s_1}\ket{s_2} \), which is factorizable if and only if the wave function is a product one, \( \psi(x,y) = \psi(x)\phi(y) \). When \( \psi(x,y) \) is non-factorizable the state \( \Psi_\ast \) is entangled.

In general, the three above states are entangled preventing the use of Pauli’s principle in its usual form because of the absence of one-electron states. However, a weak entanglement approximation holds in the problem. When this approximation is valid we can define partial spatial and spin properties of the electrons although the one-electron states remain undefined. In the atomic case, these partial properties are equivalent to the existence of quantum numbers. Moreover, in that approximation the states \( \Psi_\ast \) become unentangled ones and we can use Pauli’s principle. Next, we develop this argument in detail.

First of all, we introduce the definition of the weak entanglement regime. The usual description of the Helium atom considers in a first approximation the two electrons without mutual interaction. The states representing this first stage are separable, they are equivalent to the states \( \Psi \) but with the spatial part factorized: \( \psi(x,y) = \psi(x)\phi(y) \). Later, the neglected mutual interaction is taken into account as a perturbation, giving accurate energy levels. The ability of the method to correctly reproduce the atomic structure shows the validity of the approach and, in particular, of the use of product spatial wave functions in these cases. The spatial entanglement must be weak in order to write the wave function in a product form. Then we can denote this method as the weak entanglement approximation.

When the approximation holds the \( \Psi \)'s can be expressed in the (unnormalized) form \( \Psi_\pm \sim (\psi(x)\phi(y) \pm \psi(y)\phi(x)\ket{s_1} \ket{s_2} \pm \ket{s'_{12}} \ket{s_{12}} \) and \( \Psi_\ast \sim (\psi(x)\phi(y) - \psi(y)\phi(x))\ket{s_1} \ket{s_2} \). According to the criterion of [2] the spatial and spin parts of these states are not entangled [9] (although the
full states $\tilde{\Psi}_\pm$ are entangled). Then, following the argumentation in [2], we can attribute spatial and spin properties to the parts of the system by separate. We can say that one of the particles (we do not know which one) possesses the spatial properties associated with the one-electron wave function $\tilde{\psi}$, and the other those of $\phi$. Similarly, with respect to the spin variables, we can say that one electron possesses the spin projection $s$, and the other the $s'$ projection (for $\tilde{\Psi}_+$), or the $s$ projection (for $\tilde{\Psi}_\pm$). We remark that for the states $\tilde{\Psi}_\pm$ we can define properties for the spatial and spin variables but we cannot define a complete set of properties for each one of the particles. For instance, for $\tilde{\Psi}_-$, we have simultaneously the options for one of the particles of possessing the properties of state $\psi$, with spin projections $s$ or $s'$. We cannot attribute simultaneously spatial and spin properties to the particle. The attribution of properties is to the spatial and spin parts of the system, or, equivalently, to the two-particle system. This attribution of properties is objective in the sense used in this paper [10].

The possibility of attributing to the system the properties associated with spatial wave functions implies that we can define the usual quantum numbers $(n,l,m_l)$. Similarly, for the spin variable it is justified the definition of a spin projection (the other usual quantum number $m_s$). It must be stressed that we do not have a complete set of quantum numbers for each particle. One of the electrons in $\tilde{\Psi}_-$ (we do not know which one) is spatially characterized by $n,l,m_l$ and the other by $n',l',m_{l'}$. In the same way, one of them possesses the property $m_s$ and the other the $m_{s'}$ one. However, we cannot say if the particle with the numbers $n,l,m_l$ is in the spin projection $m_s$ or in the $m_{s'}$ one. We only can assert that the two-particle state possesses the set of quantum numbers $n,l,m_l,n',l',m_{l'},m_s,m_{s'}$. The set of quantum numbers is a property of the entangled two-electron state, not from the individual electrons.

The situation is different for $\tilde{\Psi}_+$, where we can define complete sets of properties for the particles. Each particle possesses a defined set of quantum numbers and, moreover, a defined state. This is a natural consequence of the fact that $\tilde{\Psi}_+$ corresponds to the antisymmetrization of a product state and is, consequently, non-entangled. Now, we can justify the use of Pauli’s principle in the Helium atom. It can be applied, within the weak entanglement approximation, to all the states of the form $\tilde{\Psi}_+$. It excludes these states when all the quantum numbers are equal. The exclusion of all the states $\tilde{\Psi}_+$ with equal quantum numbers is a necessary condition to theoretically explain the observed level structure of the Helium. The states $\tilde{\Psi}_+$ are only present in the structure of the atom when some of the quantum numbers of $\phi$ differ from those of $\psi$, for instance in the archetypical ortho-Helium state.
4 Excluded states with strong entanglement

When the weak entanglement approximation does not hold the Pauli principle does not make sense and we must deal with the problem of exclusion in a different way. Now, we are in the regime of strong entanglement, where any reference to the states of the constituents is misleading. In this section we show that the mathematical definition of excluded states can be extended to the strong regime and present some examples of these states.

The definition of excluded states (when Pauli’s principle can be applied) can be done in terms of their mathematical properties. Let us consider the general two-fermion antisymmetrized state

\[ \frac{|\psi >_1 |\phi >_2 - |\phi >_1 |\psi >_2}{(2 - 2 < \psi |\phi > |\phi >^2)^{1/2}} \]  

(6)

When \( \psi = \phi \) the two-fermion state becomes an undetermined expression of the type 0/0. This is a quantitative expression of Pauli’s principle. From now on, we say that a multi-fermion state is excluded when for some condition the state becomes in the undetermined form 0/0. In the case of Pauli’s principle that condition is the equality of the individual states.

We present next some examples of these excluded states. We consider again the states \( \Psi_\pm \) and \( \Psi_* \), but now not necessarily referring to the two electrons of the Helium atom. We start with the state \( \Psi_- \). When the spatial wave function is symmetric, \( \psi(x, y) = \psi(y, x) \), the numerator and the denominator are both null (\( N_- = 1/0 \)), becoming \( \Psi_- \) undefined. Clearly this is a manifestation of an exclusion-type behavior: a condition on the state of the system precludes its preparation. The difference with product states is that now the condition does not refer to the states of the particles but to the state of the complete two-particle system. The reasoning for \( \Psi_* \) is similar. When the spatial wave function is symmetric the state is undefined.

The case \( \Psi_+ \) is different. Now, we have two possibilities. The first one is for an antisymmetric spatial wave function, \( \psi(x, y) = -\psi(y, x) \), when we obtain again an undefined state. The second possibility corresponds to equal spin projections, \( s' = s \), which also implies an undefined state. Note that in the two situations (just as for \( \Psi_- \) and \( \Psi_* \)) the exclusion conditions only refer to one of the two variables, spin or spatial ones, whereas for the standard principle the conditions always simultaneously refer to the two variables.

The generalization of excluded states is by no means restricted to two-fermion systems. We briefly discuss the general case of \( n \) identical fermions. We show that, at the level of sufficient exclusion conditions, it is only necessary to consider two-fermion symmetries. This property easily follows from a well-known textbook argument. The state of the \( n \) fermions previous to antisymmetrization is denoted by \( \chi \), from which we obtain via the usual antisymmetrization procedure the (unnormalized) state \( \varphi \). The permutation of the \( i \)
and \( j \) variables of this state leads to

\[
|\varphi(x_1, s_1; \cdots; x_i, s_i; \cdots; x_j, s_j; \cdots; x_n, s_n) > =
-|\varphi(x_1, s_1; \cdots; x_j, s_j; \cdots; x_i, s_i; \cdots; x_n, s_n) > \tag{7}
\]

The state \( \chi \) is symmetric with respect to the fermions \( i \) and \( j \) if

\[
|\chi(x_1, s_1; \cdots; x_i, s_i; \cdots; x_j, s_j; \cdots; x_n, s_n) > =
|\chi(x_1, s_1; \cdots; x_j, s_j; \cdots; x_i, s_i; \cdots; x_n, s_n) > \tag{8}
\]

When this property holds for \( \chi \) it is immediate to verify that the antisymmetrized state vanishes, \( |\varphi > = 0 \). Taking into account that in the normalized form the state reads \( |\varphi > /||\varphi > | = 0/0 \), we obtain again the undetermined expression characterizing excluded states. The above exclusion condition refers to a two-fermion symmetry of the complete multi-fermion state. This condition translates in the case of product states to the usual equality of the states of two particles: for a factorizable state, \( |\chi > = |\chi_1 > \cdots |\chi_n > \), the \( ij \)-symmetry condition is equivalent to the relation \( |\chi_i > = |\chi_j > \). The equality of states for separable systems can be seen as a particular case of the more general symmetry relation.

The two-fermion symmetry relation is a sufficient exclusion condition. Next we provide an example where it is not a necessary one. We consider the case where the spatial and spin parts of the state can be factored, \( |\varphi > = \Upsilon(x_1, \cdots, x_n)|\nu(s_1, \cdots, s_n) > \), with \( \Upsilon \) antisymmetric and \( \nu \) symmetric. The spatial wave function corresponds to the antisymmetrization of \( \xi \). If \( \xi \) is symmetric with respect to the fermions \( i \) and \( j \), \( \xi(x_1, \cdots, x_i, \cdots, x_j, \cdots, x_n) = \xi(x_1, \cdots, x_j, \cdots, x_i, \cdots, x_n) \), the state is forbidden. The \( ij \)-symmetry of the spatial wave function, not of the complete state, is a sufficient exclusion condition. Note also that once more, in contrast with the Pauli principle, it is not necessary to introduce conditions on the spin variables to exclude the state.

5 Conclusions

We have studied in this paper the meaning of exclusion in systems composed of entangled identical fermions. The impossibility of defining states for the constituents prevents the application of the usual approach based on Pauli’s principle. Only when the entanglement is weak one can work, in an approximate way, in that standard framework. In that approximation, although there are not individual states, one can define partial properties for each one of the variables involved in the problem. These partial properties are equivalent in the atomic case to the introduction of quantum numbers, justifying our argument its use in entangled systems. However, these numbers cannot be understood in the standard way. They are not the labels of one-electron properties. Instead, they characterize the multi-electron state. They allow us to classify the
different atomic states according to these labels. The other important consequence of the weak entanglement approximation is that the states $\Psi_*$ can be represented by unentangled ones $\tilde{\Psi}_*$, within the scope of Pauli’s principle. The exclusion of those with equal quantum numbers gives a consistent description of the electronic structure of the Helium.

When we do not even have the possibility of defining partial properties we must confront the problem from a different perspective. In order to replace the original idea of exclusion, we have explored a concept that can extend it. The extended excluded states, are the natural mathematical generalization of the standard principle. It refers to states that for some condition have the undefined $0/0$ form typical of Pauli-type systems (when the states of the components are equal). In the examples considered in this paper the generalized exclusion conditions are mostly associated with the symmetries of the multi-fermion state previous to antisymmetrization.

In this work we have not been only interested in the physical aspects of the problem but also in the conceptual ones. Our analysis has highlighted the advantages of studying the subject from the point of view of the properties. This approach makes clear why there are not individual states in entangled systems of identical particles, a property that precludes the individuation of the constituents. Nevertheless, the most subtle aspect of the conceptual analysis is probably the status of the sets of partial properties; we have seen that they can only be associated with the complete system not with the constituents.

We conclude that the concept of exclusion must be viewed in a different way in entangled systems. The present work is only a first contact with the problem. Many other questions must be addressed. A first obvious issue is to provide an exhaustive classification of the physical conditions that lead to undetermined states of the type $0/0$. Another line of research is to consider the possible existence of other types of forbidden states, for instance, those associated with consistency conditions related to the presence of entanglement. We expect the unexplored regime of strong entanglement to be a source of interesting novel aspects of exclusion. Independently of any future development, the results presented here show once more the importance of studying the interplay between entanglement and particle identity.

References

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Note that we symmetrize one of the parts of the state (the spatial or the spin one) and antisymmetrize the other, being the full state antisymmetric. To determine if the symmetrized part is entangled or not we must use the criterion for bosons in [2]. Then the symmetrized part is separable if and only if it can be obtained by symmetrization of a factorized product of two orthogonal states or it is the product of the same state for the two particles. In our case this is so. For the spin part of the state $\tilde{\Psi}_-$ because $s$ and $s'$ are orthogonal. Similarly, for $\tilde{\Psi}_+$, it is the product of the same state $s$. On the other hand, for the spatial part of the state $\tilde{\Psi}_+\tilde{\Psi}_+$, $\psi$ and $\phi$ are orthogonal when they correspond to different energy eigenstates. If not, they are the same state and we can apply the second part of the criterion.

In order to make this point more intuitive we consider the state $(|L>_1|R>_2 - |R>_1|L>_2)(|s>_1|s'>_2 + |s'>_1|s>_2)/2$. In the spirit of [2] the ascription of spatial properties to the two-particle system is objective when it can be corroborated by measurements. In this example simultaneous position measurements at $L$ and $R$ would certify the presence of one particle at each side. A similar argument holds for the spin variable.