A Construction of the Quantum State Space

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The first postulate of Quantum Mechanics states that a system's state is fully characterized by a vector, which is an element of an abstract space called the state space. The features of this space may vary considerably from one system to another, and even for simple systems, the physical interpretation of the state vectors is not always straightforward. This seminar aims to provide a rigorous, step-by-step construction of the quantum state space associated to real space variables, first for systems with 1 degree of freedom (one particle evolving in one dimension), and then for 3D and many-body systems. Generalized kets (non-normalizable states) are tackled from the mathematical and physical points of view. The state space associated to spin variables is introduced in a second part, allowing us to discuss the notions of quantum entanglement and indistinguishability.

INTRODUCTION

Every quantum system is completely characterized by its wavefunction Ψ , which is defined on the system's configuration space, *i.e.* the space of the system's degrees of freedom. Thus, if our system consists of one particle moving along the x-axis, then its wavefunction $\Psi(x)$ is defined over \mathbb{R} . If the same particle is allowed to move in 3 dimensions, then its wavefunction $\Psi(\vec{r})$ is now defined over \mathbb{R}^3 . For two particles moving in 3D, the wavefunction $\Psi(\vec{r}_1, \vec{r}_2)$ is defined over $\mathbb{R}^3 \times \mathbb{R}^3 = \mathbb{R}^6$. For simplicity, we begin by studying a 1D particle.

I. THE 1D PARTICLE STATE SPACE

A. The L^2 Lebesgue space

We begin by treating a system consisting of a unique particle evolving in one space dimension, noted x.

The system's state is, at each point in time, completely characterized by its wavefunction $\Psi(x)$. By Born's rule, the probability of finding the particle in an infinitesimal segment dx around the position x is $|\Psi(x)|^2 dx$, imposing the normalization condition:

$$\int_{\mathbb{R}} \mathrm{d}x \left|\Psi(x)\right|^2 = 1 \tag{1}$$

Since this integral must converge, Ψ belongs to the space \mathcal{L}^2 of square-integrable functions, which is endowed with the Hermitian product:

$$\langle \Psi_1, \Psi_2 \rangle = \int_{\mathbb{R}} \mathrm{d}x \, \Psi_1^*(x) \Psi_2(x) \tag{2}$$

However, \mathscr{L}^2 is not a complete space (see Appendix A for definitions). Moreover, since all information about the system's state can be extracted by integrating the wavefunction, then two functions Ψ_1 and Ψ_2 satisfying, for all $a, b \in \mathbb{R}$,

$$\int_{a}^{b} \mathrm{d}x \,\Psi_1(x) = \int_{a}^{b} \mathrm{d}x \,\Psi_2(x) \tag{3}$$

represent the same quantum state (Ψ_1 and Ψ_2 are said to be equal *almost everywhere*). We can build a new space L^2 by identifying the functions that are equal almost everywhere (we say L^2 is the *quotient space* of \mathcal{L}^2 by the space of functions that are almost everywhere zero). L^2 is a separable Hilbert space (again, see Appendix A).

The space \mathcal{F} of possible wavefunctions depends on the system under consideration. It can be finite- or infinitedimensional. We only impose \mathcal{F} to be a subset of L^2 and the space of twice differentiable functions (so Schrödinger's equation can be applied). Hilbert spaces have many interesting properties we like to work with, yet \mathcal{F} is not necessarily a Hilbert space. Hence, we choose in practice:

- to work in L^2 when \mathcal{F} is infinite-dimensional,
- to work in $\mathcal{F} \cong \mathbb{C}^n$ when \mathcal{F} is *n*-dimensional (every finite-dimensional Hermitian space is a Hilbert).

(The expression $E \cong F$ indicates that the spaces A and B are isomorphic, hence they possess the same structure and may be considered identical.) It is possible to work in L^2 by default because \mathcal{F} is a subset thereof anyway.

B. Dual space and generalized wavefunctions

As is shown in Appendix B, it is interesting in practice to describe some systems using functions that do not belong to the Hilbert space, but extend it.

This first step in building this extension of the Hilbert space is to consider its dual spaces, which we must define. The *algebraic dual* is the space of all linear forms on a vector space. The *topological dual* is the space of continuous linear forms, and has a very important property:

Fréchet-Riesz Theorem. Every Hilbert space is isometrically isomorphic to its topological dual.

In other words, for every continuous linear form $\tilde{\psi}$ defined on a Hilbert space \mathcal{H} , there exists a unique vector ψ such that:

$$\forall \phi \in \mathcal{H} \quad \hat{\psi}(\phi) = \langle \psi, \phi \rangle \tag{4}$$

and furthermore $\|\psi\| = \|\tilde{\psi}\|$, where the norm on the topological dual \mathcal{H}' is the norm subordinate to the norm on \mathcal{H} :

$$\|\tilde{\psi}\| \stackrel{\text{def}}{=} \sup_{\{\phi \in \mathcal{H} : \|\phi\|=1\}} \left\{ \tilde{\psi}(\phi) \right\}$$
(5)

Thus, \mathcal{H}' is simply the "mirror" of \mathcal{H} . This is the justification for the use of Dirac notation, in which the mapping $\psi \mapsto \tilde{\psi}$ is written $|\psi\rangle \mapsto \langle \psi|$. There is no ambiguity in this notation since this correspondence is bijective according to the Fréchet-Riesz theorem. From a physical point of view, this justifies that $|\psi\rangle$ and $\langle \psi|$ represent the same quantum state, and that the distinction between the two is purely mathematical.

In finite dimensions, the algebraic dual \mathcal{H}^* is equal to the topological dual \mathcal{H}' . In infinite dimension, however (and in particular for L^2), there exist non-continuous linear forms, which consequently are not normalizable (the supremum in equation (5) does not exist). Since these are linear forms, they can still be applied to functions $\phi \in L^2$, and this is denoted as a scalar product: $\Phi(\phi) \stackrel{\text{def}}{=} \langle \Phi, \phi \rangle$ by analogy with equation (4). We "forget", so to speak, that Φ is a linear form that does not correspond to any wavefunction, because there is meaning in calculating its "scalar product" with a wavefunction ϕ . For every non-continuous linear form on L^2 , we thus define a *generalized wavefunction*, which is not a square-integrable function (and sometimes not even a function). For instance, the Dirac distribution

$$\langle \delta_a, \phi \rangle \stackrel{\text{def}}{=} \phi(a) \tag{6}$$

is a non-continuous linear form [1]. We associate it with the generalized wavefunction $x \mapsto \delta(x-a)$. As explained before, this only makes sense because we can compute its "scalar product" with a true (normalizable) wavefunction $\phi \in L^2$:

$$\int \mathrm{d}x \,\phi(x)\delta(x-a) \stackrel{\text{def}}{=} \langle \delta_a, \phi \rangle \tag{7}$$

In Dirac notation, this distribution is denoted $\langle x |$, and the associated generalized wavefunction becomes the *generalized ket* $|x\rangle$. Generalized kets are not elements of the Hilbert space since they are not normalizable, and their scalar product with another generalized ket is not defined *a priori*. Figure 1 illustrates that the "total" state space, often denoted \mathcal{G} , includes both the Hilbert space of normalizable states and the generalized kets defined by the non-continuous bras to which they are associated.



FIG. 1: The Hilbert space \mathcal{H} contains the normalizable kets, to which the continuous bras (the elements of \mathcal{H}') are associated. Then, to each non-continuous bra (the elements of \mathcal{H}^*), a ket is associated that lies outside of \mathcal{H} , and is called a *generalized ket* (element of \mathcal{G}).

If we want generalized kets (or generalized wavefunctions) to be of any use, we need to give meaning to their scalar product with other kets (or functions). Let $|\phi\rangle$ be a normalizable ket, then by definition we have:

$$\langle x|\phi\rangle \stackrel{\text{def}}{=} \phi(x)$$
 (8)

To generalize the properties of the Hermitian scalar product on L^2 , we define:

$$\langle \phi | x \rangle \stackrel{\text{def}}{=} \phi^*(x) \tag{9}$$

Moreover, we expect the $\{|x\rangle\}$ to form a basis of L^2 since, by virtue of equation (8), their application to a function ϕ allows us to fully characterize this function. Consequently, we want them to satisfy the closure identity:

$$\hat{\mathbb{I}} = \int \mathrm{d}x' \, |x'\rangle\!\langle x'| \tag{10}$$

and in particular:

$$|x\rangle = \int \mathrm{d}x' \,|x'\rangle \,\langle x'|x\rangle \tag{11}$$

The only way to satisfy this condition is to prescribe:

$$\langle x'|x\rangle \stackrel{\text{def}}{=} \delta(x-x') \tag{12}$$

Important Remark. We said earlier that generalized wavefunctions are not normalizable, in the sense that, not being continuous, the supremum in equation (5) is never reached. Yet, one might think that this impossibility can be circumvented using rule (12), which makes us want to write $\langle x|x \rangle = \delta(x-x) = \delta(0)$. This expression makes absolutely no sense! In accordance with definition (7), the pseudo-function $\delta(x)$ only makes sense if it can be integrated, as this amounts to applying Dirac's *delta distribution*, which is a well-defined mathematical object. In other words, we are allowed to write $\delta(x)$ only on the condition that x is an integration variable, but there is absolutely no meaning in trying to evaluate δ at a particular point.

It follows that the expression $\langle x|x\rangle$ means nothing, that $|x\rangle$ is not normalizable, and that everyone is very happy.

Finally, we define the distribution $\langle p |$ as the Fourier transform of the Dirac distribution $\langle x |$, then associate it with a generalized ket $|p\rangle$, and we can compute $\langle x | p \rangle \propto e^{ipx/\hbar}$, which means that the generalized function associated with $|p\rangle$ is the plane wave with wavenumber $\frac{p}{\hbar}$.

C. Dirac's formalism

As mentioned in the introduction, the wavefunction is defined on the system's configuration space. In all that has preceded, we have assumed that this configuration space was 1-dimensional, meaning we considered a single particle with only one degree of freedom. Nevertheless, all the mathematical results remain valid for a wavefunction defined on \mathbb{R}^n , that is, for a system with *n* degrees of freedom. In particular, it is true we can always work in a separable Hilbert space.

To reason with the most generality and simplify the notation, we consider we are working in an abstract separable Hilbert space \mathcal{H} , whose elements are the *kets* denoted $|\Psi\rangle$. We "forget", so to speak, that these state vectors are initially functions. Separability ensures that, if \mathcal{H} is infinite-dimensional, then it is isometrically isomorphic to L^2 . If \mathcal{H} is finite-dimensional, it is separable anyway, so we do not lose generality.

The space \mathcal{G} of generalized kets is never explicitly mentioned in practice. We simply speak of the state space \mathcal{H} , but it is important to keep in mind that generalized kets are always present and that we are always likely to use them.

II. PRODUCT SPACES

A. Definition and properties of tensor products

Let *E* and *F* be two vector spaces. We call **tensor product space**, and denote by $E \otimes F$, the vector space generated by all pairs (x, y) (denoted $x \otimes y$) where $x \in E$ and $y \in F$, with the following rules for defining scalar multiplication and addition:

$$\lambda(x \otimes y) \stackrel{\text{def}}{=} (\lambda x) \otimes y \stackrel{\text{def}}{=} x \otimes (\lambda y) \tag{13}$$

$$x \otimes (y_1 + y_2) \stackrel{\text{def}}{=} x \otimes y_1 + x \otimes y_2 \quad ; \quad (x_1 + x_2) \otimes y \stackrel{\text{def}}{=} x_1 \otimes y + x_2 \otimes y \tag{14}$$

Thus, the tensor product behaves like a multiplication in the usual sense.

It is important to note that not all elements of $E \otimes F$ can be written as products $x \otimes y$. Indeed, the sum $x_1 \otimes y_1 + x_2 \otimes y_2$ is generally not simplifiable, and must remain written as a linear combination of tensor products.

Because of this, to obtain a basis for $E \otimes F$, we must form all possible tensor products between the vectors $|e_i\rangle$ of a basis of E and the vectors $|f_j\rangle$ of a basis of F. The product kets $|ij\rangle = |e_i\rangle \otimes |f_j\rangle$ thus form a basis for $E \otimes F$. The symbol \otimes is usually omitted in tensor products between kets, and we write: $|ij\rangle = |e_i\rangle |f_j\rangle$. This means the dimensions multiply in a tensor product: dim $(E \otimes F) = \dim E \times \dim F$.

Let \hat{A} be an operator on E, and \hat{B} an operator on F. We can then form an operator $\hat{A} \otimes \hat{B}$ that acts on $E \otimes F$ (take $|\psi_1\rangle \in E$ and $|\psi_2\rangle \in F$):

$$(\hat{A} \otimes \hat{B})(|\psi_1\rangle |\psi_2\rangle) = (\hat{A} |\psi_1\rangle)(\hat{B} |\psi_2\rangle) \tag{15}$$

It is customary to extend \hat{A} (resp. \hat{B}) to $E \otimes F$ by identifying $\hat{A} = \hat{A} \otimes \hat{\mathbb{I}}_F$ (resp. $\hat{B} = \hat{\mathbb{I}}_E \otimes \hat{B}$), where $\hat{\mathbb{I}}_F$ is the identity tensor on F (resp. $\hat{\mathbb{I}}_E$ the identity tensor on E). We then have:

$$\hat{A}\hat{B} = (\hat{A}\otimes\hat{\mathbb{I}}_F)(\hat{\mathbb{I}}_E\otimes\hat{B}) = (\hat{A}\hat{\mathbb{I}}_E)\otimes(\hat{\mathbb{I}}_F\hat{B}) = \hat{A}\otimes\hat{B} = (\hat{\mathbb{I}}_E\otimes\hat{B})(\hat{A}\otimes\hat{\mathbb{I}}_F) = \hat{B}\hat{A}$$
(16)

Thus, two operators defined on different spaces always commute.

If E and F are pre-Hilbert spaces, then the inner product also extends to $E \otimes F$:

$$(\langle \phi_1 | \langle \phi_2 | \rangle (|\psi_1\rangle | \psi_2\rangle) = \langle \phi_1 | \psi_1 \rangle \langle \phi_2 | \psi_2 \rangle \tag{17}$$

B. Many degrees of freedom state spaces

We study the tensor product because of one fundamental property:

$$L^{2}(\mathbb{R}^{n+m}) = L^{2}(\mathbb{R}^{n}) \otimes L^{2}(\mathbb{R}^{m})$$
(18)

where $L^2(E)$ denotes the space of square-integrable functions defined on E. Notably, if we now consider a particle moving in 3D, its wavefunction $\psi(\vec{r})$ is a square-integrable function on \mathbb{R}^3 . We then have:

$$L^{2}(\mathbb{R}^{3}) = L^{2}(\mathbb{R}) \otimes L^{2}(\mathbb{R}) \otimes L^{2}(\mathbb{R}) = L^{2}(\mathbb{R})^{\otimes 3}$$

$$\tag{19}$$

Notably, a basis for the state space of a 3D particle can be obtained by forming all possible tensor products between the three basis vectors of the 1D particle state space:

$$\left|\vec{r}\right\rangle = \left|x, y, z\right\rangle = \left|x\right\rangle \left|y\right\rangle \left|z\right\rangle \tag{20}$$

Now, imagine that the system is in a state $|\psi\rangle = |u\rangle |v\rangle |w\rangle$. We can then write:

$$\psi(\vec{r}) = \langle \vec{r} | \psi \rangle = \langle x | u \rangle \langle y | v \rangle \langle z | w \rangle = u(x)v(y)w(z)$$
(21)

Saying that a state factorizes into a tensor product means that its wavefunction separates into a product of functions of the different degrees of freedom of the system. Such a state is called *separable* or *factorizable*.

More generally, a system with n degrees of freedom admits a wavefunction in

$$L^2(\mathbb{R}^n) = L^2(\mathbb{R})^{\otimes n} \tag{22}$$

For example, the simplest way to represent a system of two particles is to use a Hartree product, i.e., a separable state in the tensor product of two single-particle states, which in terms of wavefunctions gives: $\psi(\vec{r}_1, \vec{r}_2) = \psi_1(\vec{r}_1)\psi_2(\vec{r}_2)$. This form is justified if we denote $\hat{H} = \hat{H}_1 + \hat{H}_2$ as the total Hamiltonian of the system, where \hat{H}_1, \hat{H}_2 are the Hamiltonians of each of the two particles taken individually. Because they act on different spaces (since they correspond respectively to \vec{r}_1 and \vec{r}_2 , different degrees of freedom of the total system), \hat{H}_1 and \hat{H}_2 commute. Consequently, they have a common eigenbasis. Conversely, it is easy to show that a Hartree product is an eigenstate of \hat{H} : consider $|\psi_1\rangle$ an eigenket of \hat{H}_1 associated with energy E_1 and $|\psi_2\rangle$ an eigenket of \hat{H}_2 associated with energy E_2 :

$$\hat{H} |\psi_1\rangle |\psi_2\rangle = (\hat{H}_1 |\psi_1\rangle) |\psi_2\rangle + |\psi_1\rangle (\hat{H}_2 |\psi_2\rangle) = (E_1 + E_2) |\psi_1\rangle |\psi_2\rangle$$
(23)

Thus, the eigenstates of \hat{H} are indeed the tensor products of eigenstates of \hat{H}_1 and \hat{H}_2 . But beware: this form assumes no interaction between the two particles. The total Hamiltonian should in general be written as $\hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_I$ where the interaction term depends on both \vec{r}_1 and \vec{r}_2 and consequently does not commute with the other two. All we can say about the eigenstates of \hat{H} in general is that they are linear combinations of tensor products of particle 1 and particle 2 states.

An *entangled state* is a state that is not separable, a state that is written only as a linear combination of separable states. Examples of entangled states will be given in the section dedicated to spin.

C. Applications to the hydrogen atom

The hydrogen atom is a two-particle system (the proton and the electron) interacting through an electrostatic potential. By canonical reduction of the two-body system, the Hamiltonian is put in the form

$$\hat{H} = \hat{H}_{\vec{r}} + \hat{H}_{\vec{R}} \tag{24}$$

where each of the two terms depends on a different variable, the radius vector of the center of mass \vec{R} or the position of the reduced mass \vec{r} . This form leads us to write the state space of the hydrogen atom as a product:

$$\mathcal{H} = \mathcal{H}_{\vec{r}} \otimes \mathcal{H}_{\vec{R}} \tag{25}$$

where each of the two spaces $\mathcal{H}_{\vec{r}}$, $\mathcal{H}_{\vec{R}}$ corresponds to three different degrees of freedom (the position of the reduced mass and that of the center of mass, respectively). Since $\hat{H}_{\vec{r}}$ and $\hat{H}_{\vec{R}}$ act on $\mathcal{H}_{\vec{r}}$ and $\mathcal{H}_{\vec{R}}$ respectively, they commute

with each other, and we seek an eigenbasis of \hat{H} in the form of tensor products of eigenkets of one and the other. $\hat{H}_{\vec{R}}$ is the Hamiltonian of a free particle, so its eigenfunctions are plane waves; it is then necessary to diagonalize the reduced Hamiltonian $\hat{H}_{\vec{r}}$. This Hamiltonian commutes with \hat{L}^2 and \hat{L}_z , which depend on the spherical coordinates θ and φ . We decompose, again:

$$\mathcal{H}_{\vec{r}} = \mathcal{H}_r \otimes \mathcal{H}_{\theta,\varphi} \tag{26}$$

We then seek the eigenkets in the form $|\psi_r\rangle |lm\rangle$, where the $|lm\rangle$ are the common eigenstates of \hat{L}^2 and \hat{L}_z , which constitute a basis of $\mathcal{H}_{\theta,\varphi}$, and $|\psi_r\rangle \in \mathcal{H}_r$. In other words, the eigenfunctions of the reduced Hamiltonian are written as products of a radial function and a spherical harmonic.

III. SPIN STATES

A. Pauli's theory of spin

Spin is an intrinsic degree of freedom of quantum systems. Consequently, to account for it, we must take the tensor product of the orbital state space \mathcal{H}_o , the space of spatial wavefunctions that we have manipulated so far, with a new space \mathcal{H}_s , the space of spin states:

$$\mathcal{H} = \mathcal{H}_o \otimes \mathcal{H}_s \tag{27}$$

Spin as a physical quantity is described by a vector observable \vec{S} that acts on \mathcal{H}_s . It is an angular momentum, which means that S_x , S_y , and S_z obey the following commutation relations (where ε_{ijk} denotes the Levi-Civita symbol):

$$[S_i, S_j] = i\hbar\varepsilon_{ijk}S_k \tag{28}$$

In particular, the operators \hat{S}^2 and \hat{S}_z commute and thus possess a common eigenbasis $|s m_s\rangle$, where s denotes the spin quantum number and m_s the magnetic spin quantum number [2]:

$$\hat{S}_z \left| s \, m_s \right\rangle = \hbar m_s \left| s \, m_s \right\rangle \tag{29}$$

$$\hat{S}^2 |s \, m_s\rangle = \hbar^2 s(s+1) |s \, m_s\rangle \tag{30}$$

s can only take positive integer or half-integer values; the different possible values of m_s differ by an integer and are bounded by $-s \le m_s \le s$. Quantum systems with integer spin are called bosons, and those with half-integer spin are called fermions.

The electron, in particular, is a particle with spin s = 1/2. The spin state space of an electron is therefore 2dimensional, generated by the two kets: the *spin down* state $\left|\frac{1}{2} - \frac{1}{2}\right\rangle$ and the *spin up* state $\left|\frac{1}{2} + \frac{1}{2}\right\rangle$, often denoted $|-\rangle$ and $|+\rangle$, or $|\downarrow\rangle$ and $|\uparrow\rangle$ respectively.

Since these two states form a basis of \mathcal{H}_s , the total state of the electron can be written as $|\psi\rangle = |\psi_+\rangle |\uparrow\rangle + |\psi_-\rangle |\downarrow\rangle$, where $|\psi_+\rangle$ and $|\psi_-\rangle$ are orbital states, elements of \mathcal{H}_o . It can also be written in the form of a wavefunction $\psi(\vec{r},\varepsilon) = \psi_+(\vec{r})\frac{1+\varepsilon}{2} + \psi_-(\vec{r})\frac{1-\varepsilon}{2}$, where ψ_+ and ψ_- are spatial wavefunctions, and ε is a discrete variable that can take the values +1 or -1.

Performing a measurement of the electron magnetic spin number amounts to projecting $|\psi\rangle$ onto an eigenstate of \hat{S}_z , i.e., applying one of the following projectors:

$$\hat{P}_{+} = \int \mathrm{d}^{3}\vec{r} \, |\vec{r}\rangle \, |\uparrow\rangle\langle\vec{r}| \, \langle\uparrow| = \int \mathrm{d}^{3}\vec{r} \, |\vec{r}\rangle\langle\vec{r}| \otimes |\uparrow\rangle\langle\uparrow| \tag{31}$$

$$\hat{P}_{-} = \int \mathrm{d}^{3}\vec{r} \, |\vec{r}\rangle \, |\downarrow\rangle\langle\vec{r}| \, \langle\downarrow| = \int \mathrm{d}^{3}\vec{r} \, |\vec{r}\rangle\langle\vec{r}| \otimes |\downarrow\rangle\langle\downarrow| \tag{32}$$

The probability of measuring the electron in the spin-up state is therefore $\langle \psi | \hat{P}_+ | \psi \rangle = \int d^3 \vec{r} |\psi_+(\vec{r})|^2$, and in the spin-down state $\langle \psi | \hat{P}_- | \psi \rangle = \int d^3 \vec{r} |\psi_-(\vec{r})|^2$.

To simplify the writing of the electron wavefunction and focus on its spatial dependence, it is customary to write it in the form:

$$\psi(\vec{r}) = \begin{bmatrix} \psi_+(\vec{r}) \\ \psi_-(\vec{r}) \end{bmatrix}$$
(33)

Such an object is called a *Pauli spinor*.

в. Spin of the two-electron system: indistinguishability and entanglement

Let us now study the spin states accessible to a system of two electrons. The spin space of the system is none other than the tensor product $\mathcal{H}_{s1} \otimes \mathcal{H}_{s2}$ of the spin spaces of each of the two electrons. It is therefore a 4-dimensional space, for which we can provide a basis of product states: $|\uparrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$, $|\downarrow\downarrow\rangle$, $|\downarrow\downarrow\rangle$ (where $|\uparrow\uparrow\rangle = |\uparrow\rangle |\uparrow\rangle$, etc.). However, these kets are not necessarily eigenstates of \hat{S}^2 , where $\hat{\vec{S}} = \hat{\vec{S}}_1 + \hat{\vec{S}}_2$ is the total spin observable. It is not very difficult to diagonalize \hat{S}^2 , which gives the following eigenbasis (S and M_S denote the total spin

quantum number and the total magnetic spin quantum number, respectively):

$$|S=0, M_S=0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$
(34)

$$|S = 1, M_S = 1\rangle = |\uparrow\uparrow\rangle \quad , \quad |S = 1, M_S = 0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \quad , \quad |S = 1, M_S = -1\rangle = |\downarrow\downarrow\rangle \tag{35}$$

The first state (with spin 0) is called a singlet state. The following three states (with spin 1) are called triplet states. Unlike the product states, these eigenstates are either symmetric (the triplet) or antisymmetric (the singlet) under the exchange of the two electrons. This is explained by the indistinguishability of particles: unlike two classical particles whose trajectories can be followed, two identical quantum particles cannot be labeled, since their wavefunctions "mix" completely (this is still a naive description: the "two wavefunctions" do not actually mix since there is only one wavefunction for the whole system).

Performing a measurement of S or M_S (thus projecting the system into an eigenstate) should not allow the two electrons to be distinguished. If $|\uparrow\downarrow\rangle$ were an eigenstate into which the system was projected, one could say upon seeing the measurement result, "the spin of electron 1 is up and the spin of electron 2 is down".

For two of the eigenstates (those with magnetic number 0), indistinguishability is ensured by the fact that these are entangled (non-separable) states. This is again a purely quantum phenomenon: the two electrons can be very far apart, but if the spin of one is measured, the spin of the other is instantly determined.

For example, suppose the system is in the state $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$, but the two electrons are now spatially separated. We measure the spin of the first electron and find it to be up (there is a 50% chance). The system is projected into the state $|\uparrow\downarrow\rangle$, so despite the distance separating them, the spin of the second electron instantly becomes down.

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Appendix A: Reminders of linear algebra and related topology

A metric space is a vector space endowed with a distance, so the notion of *limit* is well-defined.

F is called a dense subset of E if each vector in E is the limit of a certain sequence of elements of F. A topological space is termed *separable* if it contains a dense countable subset. The separability of a Hilbert space ensures the existence of a Hilbert basis, even when the space is infinite-dimensional. A Hilbert basis is the generalization to infinite-dimensional spaces of orthonormal bases: each vector in the Hiblert space can be uniquely decomposed as a series of weighted elements of the Hilbert basis, and the basis elements are unitary and orthogonal to one another.

A Cauchy sequence is a sequence in which the elements are all progressively getting arbitrarily close to one another, so that every converging sequence is also a Cauchy sequence. A metric space is said to be *complete* if every Cauchy sequence converges in it. Morally, it is a space where all holes have been "filled": \mathbb{Q} is not complete, but \mathbb{R} is. \mathbb{R} is constructed by adding to \mathbb{Q} the limits of all rational Cauchy sequences, *i.e.* by completing \mathbb{Q} .

Appendix B: Discrete and continuous spectra

This appendix is a discussion on the nature of the Hamiltonian's spectrum, where we justify the use of nonnormalizable functions. Let us consider a particle of mass m evolving in a 1-dimensional potential V(x), such that $V(x) \xrightarrow[x \to \infty]{} V_{\infty}$. The quantum-mechanical problem consists in solving the stationary Schrödinger equation:

$$\frac{-\hbar^2}{2m}\nabla^2\phi(x) + V(x)\phi(x) = E\phi(x)$$
(B1)

which becomes at infinity:

$$\nabla^2 \phi(x \to \infty) + \frac{2m}{\hbar^2} (E - V_\infty) \phi(x \to \infty) = 0$$
(B2)

To solve this asymptotic Schrödinger equation, we need to distinguish between the possible energy regimes:

- if $E < V_{\infty}$, then $\phi(x) \underset{x \to \pm \infty}{\sim} \exp\left(\mp \frac{\sqrt{2m(V_{\infty} E)}}{\hbar} x\right);$
- if $E > V_{\infty}$, then $\phi(x) \underset{x \to \pm \infty}{\sim} \exp\left(\mp i \frac{\sqrt{2m(E-V_{\infty})}}{\hbar}x\right)$.

The first case is that of a bound state, where a classical particle would be trapped in the potential. ϕ is a vanishing wave, so the quantum particle can escape, but with an exponentially decreasing probability, and a penetration length proportional to the particle's de Broglie wavelength $\lambda = h/\sqrt{2m(V_{\infty} - E)}$. The exponential damping ensures the normalizability of the wavefunction; in this case, the spectrum is discrete and the energy eigenstates are Hilbert space kets.

The second case is that of a scattering state, where a classical particle is able to escape the potential. ϕ is a plane wave, so the quantum particle is delocalized at infinity, and is better described as a probability current proportional to the particle's de Broglie frequency $\nu = v/\lambda$. Such a function is not normalizable; in this case, the spectrum is continuous and the energy eigenstates are generalized kets.

This simple but very general argument shows that generalized kets (such as plane waves or Dirac deltas) are necessary to correctly describe quantum scattering states.

Of course, such generalized wavefunctions are not physical states, but physical (normalizable) states can be formed as wavepackets, superpositions of generalized wavefunctions.

[4] G. B. Arfken, H. J. Weber, and F. E. Harris, *Mathematical methods for physicists* (Elsevier Academic Press, 2013).

^[1] The Dirac distribution is not continuous on L^2 , but it is continuous on the space \mathcal{D} of test functions, whose topology is different.

^[2] In practice, both s and m_s are called "spin" when there is no ambiguity. s is characteristic of the type of particle, whereas m_s is characteristic of a given particle. Therefore, when we say "electrons are spin-1/2 particles", we are referring to s, but when we say "this photon is of spin +1/2", we are referring to m_s .

^[3] C. Cohen-Tannoudji, B. Diu, and F. Laloë, Mécanique quantique I (Hermann, 1977).