Visualizing the Origin of the Exchange Energy

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Abstract Atoms and molecules with two unpaired electrons can adopt singlet and triplet spin multiplicities. The implications of this are far reaching. For instance, the properties of molecular oxygen with its triplet ground state cannot be understood if this is not considered. In the design of emitters for OLEDs, the energy gap between singlet and triplet excitations is of utmost importance. This energy gap equals twice the exchange energy. Because of this relevance, the exchange energy is treated in textbooks and courses on physical and quantum chemistry. The treatments are commonly based on the quantum mechanical formalism and leave the students wondering why the exchange energy is non-zero. Here, the formalism is briefly re-iterated. Then wavefunctions for singlet and triplet states with identical configurations are visualized relying on the well-known particle-in-a-box model. The visualization shows that in the triplet state the electrons "automatically" avoid each other. This lowers the triplet energy compared to the singlet one. Some short comings of this didactic approach are also discussed.

Keywords: upper-division undergraduate, chemistry bachelor programs in Europe, physical chemistry, quantum chemistry, photochemistry, exchange energy, particle-in-a-box model

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1. Introduction

Atoms and molecules may possess two unpaired electrons. A prominent example for a molecule with two unpaired electrons in the electronic ground state is molecular oxygen, O_2 [1]. Molecules with only paired electrons in the ground state undergo unpairing upon photo-excitation (Figure 1) [2,3]. The spins of the two unpaired electrons may compensate each other so that a state with singlet multiplicity results. In the context of photo-excitations the respective states are termed $S_{1,2,3,...}$. For a parallel alignment of the two electron spins, states with triplet multiplicity ($T_{1,2,3...}$) result. Singlet and triplet states of a molecule even with identical orbital occupancies differ grossly in their physical and chemical properties. For instance, organic matter including ourselves persist in air despite the fact that oxygen is a very strong oxidant [4]. This kinetic stability can – at least partially – be attributed to the fact that the electronic ground state of oxygen is of triplet multiplicity [4]. Singlet states of oxygen are excited states and may be prepared chemically or photochemically [5,6]. With regards to organic matter singlet oxygen is much more reactive [7].

Singlet and triplet excitations are of paramount importance in all areas of photochemistry [2,3] and photobiology [7]. Many studies in these fields address the question whether an excited singlet or triplet state holds responsible for the photoreactivity of a molecule. For examples concerning the photoreactivity of DNA bases see ref. [8]. The topic is also of current technical interest. The emission efficiency of organic light emitting diodes (OLEDs) can be enhanced substantially by taking the spin multiplicity into account [9,10,11]. The subject, thus, deserves an extensive coverage in bachelor and master courses on physical and theoretical chemistry.

A very important physical quantity in this context is the exchange energy K. Its value is given by half the energetic separation of singlet and triplet states originating from the same orbital occupancy (cf. Figure 1) [12]. In molecular oxygen the exchange energy K is equal to 0.82 eV (79 kJ/mol) [1]. S1 and T_1 states of many aromatic molecules are separated by energies of the same magnitude [3]. These separations are in the range of chemical reaction energies [13] and, thus, by no means quantités négligeable. Physical [13], quantum [14] and photochemistry [2] textbooks treat the exchange interaction. Its physical origin is commonly explained relying on the pertinent equations. In the context of a physical chemistry lecture

for a bachelor program (according to the Bologna process [15]) we sought for a visual explanation of the exchange energy. Such a visualization was reported a few years ago using atomic orbitals [16,17]. Here, a visualization based on particles-in-a-box wavefunctions is presented. Before this visualization and its advantages are presented, a brief survey of the theoretical background will be given.
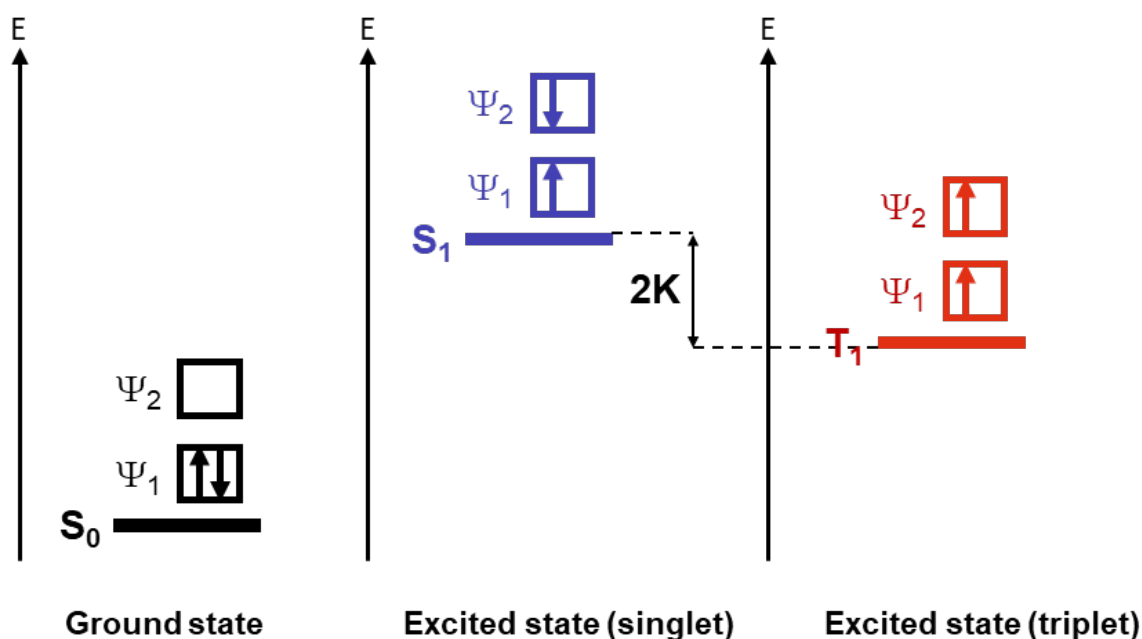

Figure 1. Energetic consequence of the exchange interaction illustrated for a molecule with a singlet ground state S_0 (left). This state features doubly occupied orbitals. The one highest in energy is denoted with ψ_1. The unoccupied orbital lowest in energy is denoted ψ_2. Excited states are formally constructed by promoting one electron from the orbital ψ_1 to the orbital ψ_2. The excitation can result in a singlet state S_1 (center) and a triplet state T_1 (right). The two excited states are energetically separated by twice the exchange energy, *2K*.

2. Two Electron Wavefunctions

The exchange interaction is relevant for all atoms and molecules containing two or more electrons. Only two electrons are considered here. The results are also relevant for atoms and molecules with more than two electrons provided that only two electrons are unpaired. In quantum mechanics the properties of these two electrons are inscribed in a two electron wavefunction $\Psi\left(\vec{r}_{s,1};\vec{r}_{s,2}\right)$. The components of the vectors $\vec{r}_{s,1,2}$ are the three spatial coordinates $x_{1,2}, y_{1,2}, z_{1,2}$ as well as the spin coordinates $\sigma_{1,2}$ of the two electrons. The absolute square of this wavefunction, $\left|\Psi\left(\vec{r}_{s,1};\vec{r}_{s,2}\right)\right|^2$, gives the probability density for the two electrons adopting the coordinates given by $\vec{r}_{s,1}$ and by $\vec{r}_{s,2}$. Since we cannot distinguish the two electrons, the absolute square must remain constant when exchanging the coordinates

$$\left|\Psi\left(\vec{r}_{s,1};\vec{r}_{s,2}\right)\right|^2 = \left|\Psi\left(\vec{r}_{s,2};\vec{r}_{s,1}\right)\right|^2. \tag{1}$$

The importance of this indistinguishability was stressed by Erwin Schrödinger: "Man kann Elektronen nicht kennzeichnen, nicht 'rot anstreichen' und nicht nur das, man darf sie sich nicht einmal gekennzeichnet *denken*, sonst erhält man durch 'falsche Abzählung' auf Schritt und Tritt falsche Ergebnisse." [18] ("One may not label electrons, not 'paint them red', and not only that, one may not even *consider* them labeled. Otherwise one obtains wrong results at every turn due to 'wrong accounting'.", translation by the authors). The fact that the absolute square needs to be invariant upon exchange leaves two possibilities (minus or plus) for the wavefunction itself. For electrons which are fermions the minus sign applies:

$$\Psi\left(\vec{r}_{s,1};\vec{r}_{s,2}\right) = -\Psi\left(\vec{r}_{s,2};\vec{r}_{s,1}\right). \tag{2}$$

The function is, thus, anti-symmetric with respect to exchange. A very important consequence of this minus sign is the Pauli exclusion principle which is the theoretical basis of the Aufbau principle of the periodic system. To arrive at singlet and triplet states we separate spatial ($\vec{r}_{1,2}$) and spin coordinates ($\sigma_{1,2}$):

$$\Psi\left(\vec{r}_1,\sigma_1;\vec{r}_2,\sigma_2\right) = -\Psi\left(\vec{r}_2,\sigma_2;\vec{r}_1,\sigma_1\right). \tag{3}$$

Commonly, the two-electron wavefunction $\Psi\left(\vec{r}_1,\sigma_1;\vec{r}_2,\sigma_2\right)$ is expressed using one-electron functions. In the simplest approximation, only two one electron functions $\psi_{1,2}$ for the spatial part and the two spin functions α and β enter the expression. These one-electron wavefunctions are usually termed atomic or molecular orbitals. Based on these orbitals one may construct two-electron functions which are anti-symmetric with respect to exchange. The resulting wavefunctions can be classified according to their overall spin S. For $S=0$ implying singlet multiplicity ($2S+1=1$) the wavefunction adopts the following form:

$$\Psi_S\left(\vec{r}_1,\sigma_1;\vec{r}_2,\sigma_2\right)=$$

$$\frac{1}{\sqrt{2}}\left(\psi_1\left(\vec{r}_1\right)\psi_2\left(\vec{r}_2\right)+\psi_2\left(\vec{r}_1\right)\psi_1\left(\vec{r}_2\right)\right)$$

$$\cdot\frac{1}{\sqrt{2}}\left(\alpha\left(1\right)\beta\left(2\right)-\beta\left(1\right)\alpha\left(2\right)\right)$$

The factors $\frac{1}{\sqrt{2}}$ in front of the brackets ensure normalization of the two-electron wavefuntion. It is crucial to realize that the spatial part of the wavefunction, i.e. the term:

$$\frac{1}{\sqrt{2}}\left(\psi_1\left(\vec{r}_1\right)\psi_2\left(\vec{r}_2\right)+\psi_2\left(\vec{r}_1\right)\psi_1\left(\vec{r}_2\right)\right)$$

is symmetric with respect to exchange; there is a plus sign in the expression. The spin part

$$\frac{1}{\sqrt{2}}\left(\alpha\left(1\right)\beta\left(2\right)-\beta\left(1\right)\alpha\left(2\right)\right)$$

is anti-symmetric. Due to the minus sign, exchanging the two electrons changes the sign of the spin part. The product of a symmetric spatial and an anti-symmetric spin part yields an anti-symmetric two-electron wavefunction.

Two-electron wavefunctions with an overall spin $S=1$ describe triplet $(2S+1=3)$ states. In the respective wavefunctions:

$$\Psi_T\left(\vec{r}_1,\sigma_1;\vec{r}_2,\sigma_2\right)=$$

$$\frac{1}{\sqrt{2}}\left(\psi_1\left(\vec{r}_1\right)\psi_2\left(\vec{r}_2\right)-\psi_2\left(\vec{r}_1\right)\psi_1\left(\vec{r}_2\right)\right) \qquad (5)$$

$$\cdot\begin{cases}\alpha\left(1\right)\alpha\left(2\right)\\ \frac{1}{\sqrt{2}}\left(\alpha\left(1\right)\beta\left(2\right)+\beta\left(1\right)\alpha\left(2\right)\right)\\ \beta\left(1\right)\beta\left(2\right)\end{cases}$$
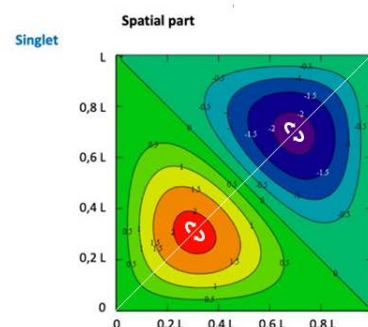
the spatial part is anti-symmetric with respect to exchange. There is a minus sign in the first bracket. Three different functions are possible for the spin part. This accounts for the orientation of the overall spin with respect to the quantization axis. All of them are symmetric with respect to exchange. So again the product of spatial and spin part is anti-symmetric. In comparison to the singlet state symmetric and anti-symmetric behavior are interchanged. The difference in the spatial part – a plus sign for the singlet and a minus sign for the triplet state – is responsible for the exchange energy.

For better understanding the above discussed equations (4) and (5) are didactically visualized in Figure 2.
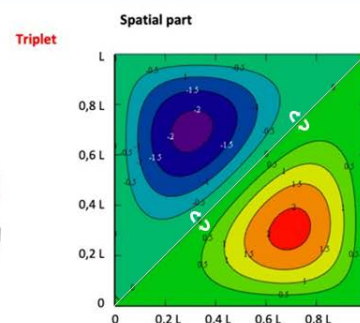

Figure 2. Correspondence between the signs in the singlet and triplet wavefunctions (eq. (4) and (5)) and the symmetry properties of the respective diagrams (for a description of these diagrams see Figure 4). The plus sign in the spatial part of the singlet wavefunction corresponds to a symmetric behavior of the respective diagram upon rotation around the diagonal. For the triplet state the minus sign corresponds to an anti-symmetric behavior

3. Simple One Electron Wavefunctions

To visualize how this seemingly "innocent" sign can have such a huge energetic effect we rely on very simple one-electron wavefunctions or orbitals most students should be familiar with. The wavefunctions are those of a particle-in-a-box (PIB). This model is often relied on in courses on quantum mechanics. It can illustrate the important quantum mechanical finding that bound particles have discrete energy levels. It is also popular to qualitatively explain trends in quantum systems. For instance, in a homologous series of molecules bearing a π-system, the red-shift of the absorption with conjugation length can be explained with the PIB approach (this application of the PIB is sometimes referred to as Kuhn model [19,20]). Also trends in the optical properties of

nanoparticles are rationalized with the PIB model (see e.g. ref. [21]). The PIB wavefunctions are also advantageous since they are mathematically simple; they are just sine functions. These wavefunctions are described by the following equation:

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n \cdot \pi \cdot x}{L}\right) \qquad (6)$$

We hereby restrict ourselves to motions in one dimension, i.e. we use one spatial coordinate x instead of the vector $\vec{r}$. The quantum number n may adopt the values 1, 2, 3, …. For the visualization we use the functions with $n=1$ and $n=2$. This relates to the orbital occupancy of the two excited state, S_1 and T_1, sketched in Figure 1. The width of the box is denoted L, i.e. $0 \leq x \leq L$. For computations we set this length to 10 Å (conjugation length of a typical chromophore), in the plots we will use a normalized length, $x_{1,2}/L$.

The PIB wavefunctions for $n=1$ and $n=2$ are plotted in Figure 3 (a Mathcad notebook, used to generate this and the following figures, can be found in the Supporting Information, SI). The function for $n=1$ is the lowest in energy and has no node. The one with $n=2$ has one node

and is higher in energy. The energy of the PIB wavefunction is given by:

$$E_n = \frac{h^2}{8m_e}\frac{n^2}{L^2} \qquad (7)$$

where h is Planck's constant and m_e the mass of the electron.

4. Visualization of Two-Electron Wavefunctions

We now have the ingredients for our visualization. The two PIB wavefunctions (eq. (6)) are inserted in the expression for the two-electron wavefunctions (eq. (4) and (5)). Of these wavefunctions we just consider the spatial part. As we restrict ourselves to motions in one dimension, we only need two spatial coordinates, x_1 and x_2, one for each electron. As the two-electron wavefunctions are real values here, simple contour representations can be used to visualize these wavefunctions (Figure 4).
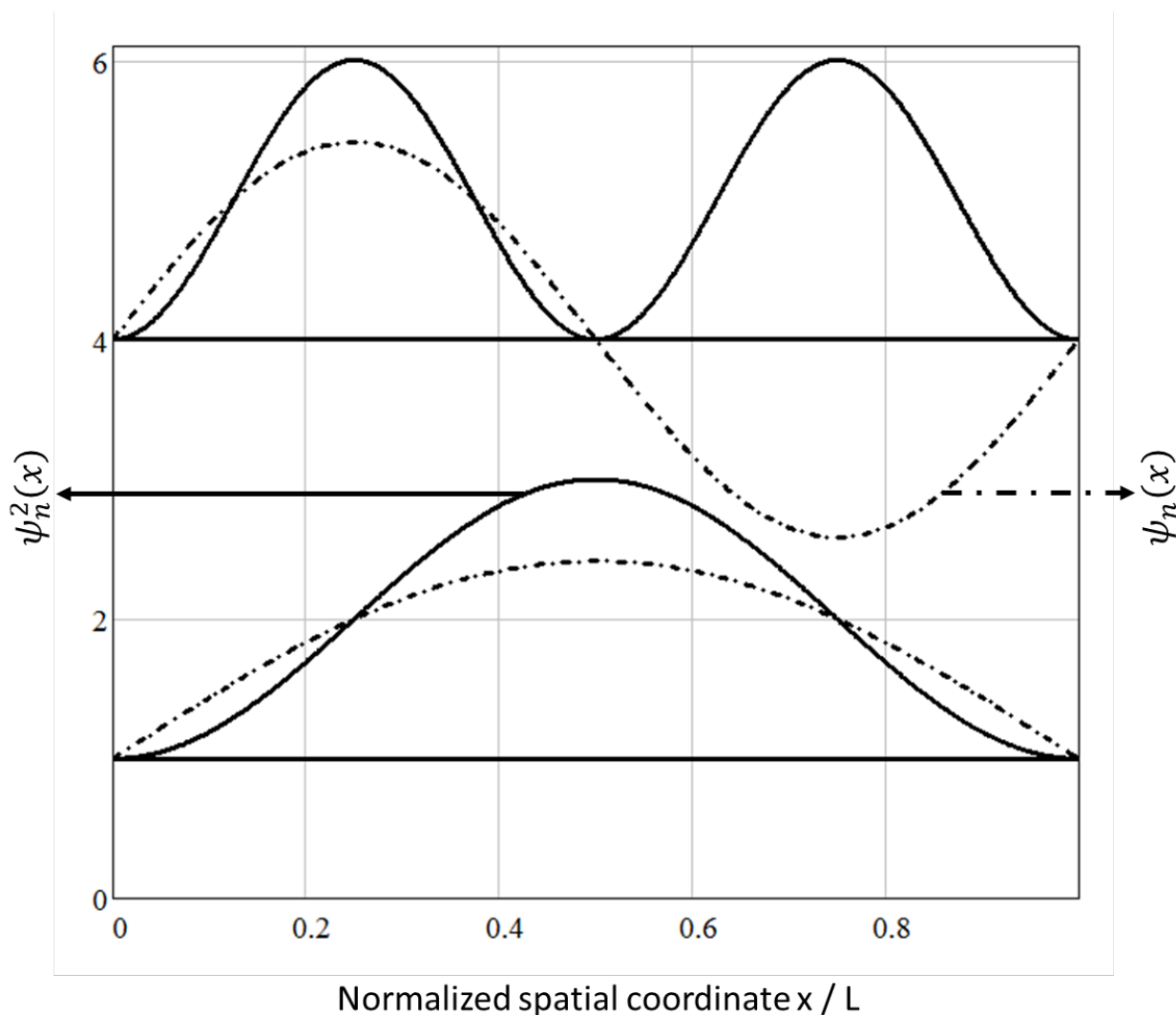

Figure 3. Lowest two ($n=1,2$) PIB wavefunctions (dash-dotted lines) and their absolute squares (solid lines). The wavefunctions and their squares have been shifted vertically according to their energy.
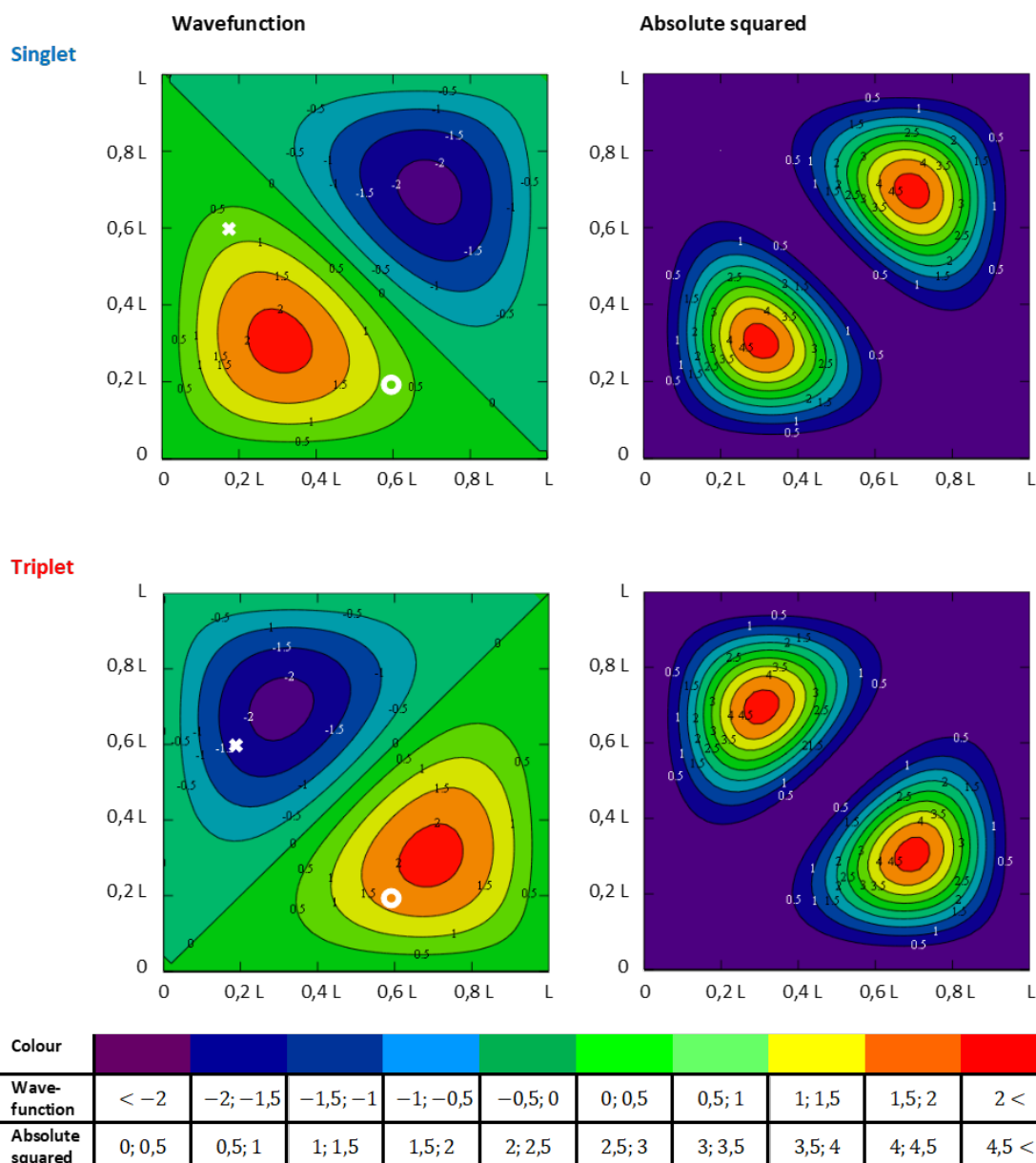
Figure 4. Contour representation of the spatial part of the two-electron wavefunction considered here (left) and their absolute square (right). The top row refers to the singlet state, the lower one to the triplet one.

Before we turn to the implications of these diagrams, we give a brief description on how to read them. The diagrams on the left represent the spatial part of the functions Ψ_S and Ψ_T. To retrieve values for certain coordinates, e.g. x_1=0.2 L and x_2=0.6 L (white crosses in the diagrams), one locates these coordinates and reads the value using the contour lines. For the singlet state a value of 0.79/L is obtained. Note that wavefunctions are related to probability densities and are therefore not dimensionless. For two electrons and one spatial coordinate the dimension of the wavefunction is a reciprocal length. Because of the symmetry issue discussed above the value at x_1=0.6 L and x_2=0.2 L (white circles) is identical to the one at x_1=0.2 L and x_2=0.6 L. For the triplet state, the same coordinates are looked upon. For x_1=0.2 L and x_2=0.6 L the value is -1,77/L. Interchanging the coordinates, i.e. x_1=0.6 L and x_2=0.2 L changes the sign to +1,77/L. This reflects the anti-symmetric nature of the spatial part of triplet

wavefunctions. In the same way, values for the absolute square can be obtained from the diagrams on right.

The effect of the exchange is directly visible in these diagrams. Exchange of the electrons is nothing else than the exchange of the two coordinates or in other words a rotation around the diagonal (see Figure 2). The diagrams giving the absolute square (Figure 4, right) are symmetric with respect to this diagonal, matching the condition given by eq. (1). The spatial part of the singlet wavefunction Ψ_S is symmetric with respect to the reflection in accordance to eq. (4). The anti-symmetric nature of the spatial part of the triplet wavefunction Ψ_T (eq. (5)) also shows up in the respective diagram.

Using these diagrams, we will now rationalize why for identical orbital occupancies singlet and triplet states differ in their energy. To this end, we inspect the diagonals of the diagrams and the regions close to these diagonals. Cuts of the diagrams in Figure 4 along the

diagonal are plotted in Figure 5. Along the diagonal the two coordinates obey $x_1=x_2$, i.e. their spatial separation is zero. Slightly above and below the diagonal the separation is small. As two electrons experience electrostatic repulsion, there is an energetic penalty for sharing the same region of space. The singlet wavefunction Ψ_S and its absolute square have non-vanishing values along the diagonal. This results in a large – in fact diverging (see below) – electrostatic repulsion. The triplet wavefunction

Ψ_T and thereby its absolute square is zero all over the diagonal and small close to it. So, in the triplet state the electrons "automatically" avoid each other. This lowers the electrostatic repulsion and explains why triplet states are lower in energy in comparison to singlet states with the same orbital occupancy. The inverted situation is observed for the "anti-diagonal", $x_2=L-x_1$. Here, the values for the singlet state vanish and those for the triplet state are non-vanishing.
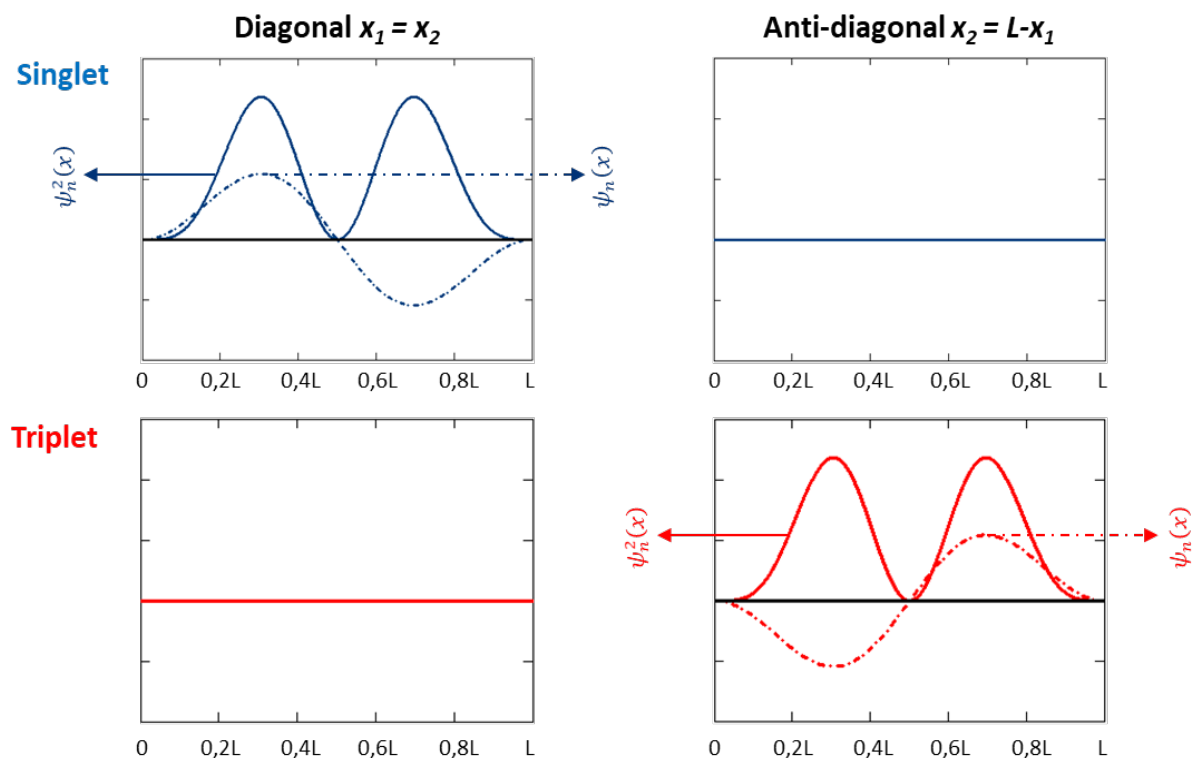

Figure 5. One dimensional cuts along the contour representations plotted in Figure 4. The graphs on the left refer to the diagonal ($x_1=x_2$), the ones on the right the "anti-diagonal" ($x_2=L-x_1$). Dash-dotted lines represent wavefunctions, the solid ones their absolute square

The diagrams also demonstrate that the nodal properties of the orbitals show up in the two-electron wavefunctions. The "orbitals" used here are PIB wavefunctions for $n=1$ (no node) and $n=2$ (one node). As consequence one nodal line is seen in the diagrams in Figure 3. It is along the anti-diagonal for the singlet wavefunction and along the diagonal for the triplet one.

5. Some Expectation Values

The diagrams in Figures 4 and 5 show clearly that the average distance of the two electrons is larger for the triplet state compared to the singlet one. We will now quantify this difference. This can also be used to familiarize students with the methods to retrieve physical information from wavefunctions. The average distances of the two electrons is the expectation value of $|x_1 - x_2|$. Expectation values are often symbolized by $<...>$ and can be expressed using Dirac's bra-ket notation or with the appropriate integrals:

$$\langle |x_1 - x_2| \rangle_{S,T} = \langle \Psi_{S,T} | |x_1 - x_2| | \Psi_{S,T} \rangle$$
$$= \iint_0^L |\Psi_{S,T}|^2 |x_1 - x_2| dx_1 dx_2 \qquad (8)$$

The double integral covers the coordinates x_1 and x_2. Each integral runs from 0 to the length L of the box. Numerical evaluation of the integrals using Mathcad yields (see SI) the expectation values for the singlet and the triplet states in multiples of box length L (eq. (9)).

$$|x_1 - x_2|_S = 0.157 \cdot L$$

$$\qquad (9)$$

$$|x_1 - x_2|_T = 0.383 \cdot L$$

The computation confirms the qualitative result of the visualization. The average distance for the triplet state is larger than the one for singlet state by more than a factor of two. As mentioned above, the difference in distance results in different electrostatic repulsions which explains

the exchange interaction. To compute the repulsion one does not average over the distance directly, but over its reciprocal. The repulsion results from the following expectation value:

$$
\left\langle \frac{e_0^2}{4\pi\varepsilon_0 |x_1 - x_2|} \right\rangle S,T
$$

$$
= \left\langle \Psi_{S,T} \left| \frac{e_0^2}{4\pi\varepsilon_0 |x_1 - x_2|} \right| \Psi_{S,T} \right\rangle \qquad (10)
$$

$$
= \iint\limits_0^L \Psi_{S,T}^2 \frac{e_0^2}{4\pi\varepsilon_0 |x_1 - x_2|} dx_1 dx_2
$$

which contains the reciprocal of the distance. e_0 represents the elementary charge and ε_0 the vacuum permittivity. For the singlet state the computation diverges, i.e. a value of $+\infty$ results. This is the consequence of the non-vanishing probability density along the diagonal in the respective diagram in Figure 3 (see also Figure 4). Along the diagonal the distance between the electrons is zero and the reciprocal thus diverges. The respective computation for the triplet state yields a finite value, given by:

$$
\left\langle \frac{e_0^2}{4\pi\varepsilon_0 |x_1 - x_2|} \right\rangle_T = 2.966 \frac{e_0^2}{4\pi\varepsilon_0} \cdot \frac{1}{L} \qquad (11)
$$

If we insert a box length L of 10 Å we obtain a repulsion energy of 4.273 eV (409 kJ/mol). This repulsion energy is much larger than the difference of the two "orbitals" energies which here amounts to only 1.128 eV (109 kJ/mol).

So, within our model and the chosen parameters, an electrostatic repulsion of $+\infty$ and 4.273 eV are computed for the singlet and triplet state, respectively. The divergence for the singlet state is a consequence of the one-dimensional nature of our model. In two or three dimensions the respective integrals yield finite values also for singlet states [22]. Though this holds true for any geometry, it is rather easy to rationalize for spherical objects like atoms. Here, the integral corresponding to eq. (10) can be computed using spherical coordinates, among them the radius r. In the respective expression the factor r^2 appears. This "removes" the singularity occurring in the one-dimensional case if the electrons are at the same location. Still, also in three dimensions, the electrostatic repulsion is higher for singlet than for triplet states. The probability of the two electrons being close to each other (and not only at the same point of space) is higher for the singlet states. This can also be perceived in our one-dimensional model (cf. Figure 4). Along the diagonal of the contour representation the distance of the two electrons is zero. Slightly above and below these diagonals their distance is small. In the areas around the diagonal, the probability density is much higher for the singlet than for the triplet state.

The large magnitude of the electrostatic repulsion, which here could only be computed for the triplet state, reminds us to be careful when filling orbitals – atomic or molecular – with electrons. Atomic orbitals appearing in common textbooks are the ones of the hydrogen atom. This atom contains only one electron. Thus, no electron-

electron repulsion has to be considered. If we now naively fill these orbitals with electrons to describe other atoms this repulsion will not be considered. The same applies for the Kuhn model for π-systems. The Kuhn model approximates molecular orbitals by PIB wavefunctions and makes no allowances for electron-electron repulsion. Not so surprisingly pathological numerical values for the repulsion result.

6. Conclusions

The electrostatic repulsion of electrons is of central importance for the energetics of atoms and molecules. Due to the Pauli principle the distribution of electrons depends on the overall spin of the system. For singlet and triplet spin states frequently encountered, differences in electron distributions can be visualized using simple particle-in-a-box wavefunctions. The respective diagrams clearly show that opposed to the singlet state, the electrons avoid each other in the triplet state. This avoidance is the origin of the exchange energy. The model can, thus, explain the origin of the exchange energy on qualitative level. Quantitatively, it fails due to its one-dimensional nature and concomitantly diverging numerical values.

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