



# A Quantum Toy-Model for Inelastic Scattering and Catalysis Based on Bäcklund Transformations

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## Abstract

This work presents a scalar self-consistent quantum model for molecular simulation. This model employs Bäcklund transformations to eliminate the wave function from Klein-Gordon and Schrödinger-type equations. The non-linear PDE obtained after coupling the quantum model with the Gauss law of electromagnetism contains only the interaction potential. The analytical solutions obtained reproduce some relevant effects related to the evolution of the electronic clouds induced by nonlinear scattering. One of the most relevant results obtained from this new formulation is to confirm and fully justify the fact that Cl<sub>2</sub> molecules do not react directly with aromatic rings. This result cannot be reproduced by classical models for molecular simulation. On the other hand, quantum chemistry only furnishes indicia that such electrophilic reactions may not occur, but does not shows explicitly how the electronic clouds evolve along the chemical process.

## Subject Areas

Combinatorial Mathematics

## Keywords

Nonlinear Quantum Models, Bäcklund Transformations, Analytical Solution

## 1. Introduction

Scattering processes and transitions between quantum states are strongly dependent phenomena usually treated as uncorrelated events. It occurs because the

coupling between quantum and electromagnetic models produces sets of high-order nonlinear partial differential equations. These equations describe the evolution of the electronic cloud of the atoms whose interaction with radiation generates scattering and electron transitions.

The most traditional quantum methods employed in molecular simulation are based on iterative schemes such as LCAO-MO and DFT formulations [1] [2] [3]. These schemes generate very accurate results in chemistry, furnishing excellent estimations for bond orders, electron densities and bond lengths for a wide class of molecules [4]. However, these variational formulations usually generate computational codes whose time processing required becomes extremely high for many important applications in Chemical and Nuclear Engineering [5]. It occurs because the total wavefunction for the chemical system consists in linear combinations containing hundreds or thousands of terms, even for relatively simple reactants. For this reason, investigating reaction mechanisms and estimating final products via quantum models often require a considerable computational effort. Moreover, the corresponding computational codes demand a time processing which grows with the square of the total number of electrons. It is important to take in mind that the total wavefunction is usually a linear combination of eigenfunctions of the Hamiltonian operator. Each eigenfunction represents a single electron, so a typical molecule of a regular organic compound must be represented by a linear combination containing thousands of basis functions.

In order to overcome this difficulty, some classical nonlinear models [6] [7] [8] generated ingenious computational codes conceived to simulate the interaction of large populations of molecules and microorganisms. Although these systems can produce important results in biological sciences and Statistical Thermodynamics, the quantum effects describing the rearranging of electronic clouds during reactions are absent in the corresponding classical models. It occurs that, in Organic Chemistry, the heart of the matter is an unexplored theme in both areas: the rearranging of electron clouds. This subject lies at the interface between classical Molecular Simulation and Quantum Physics.

For quantum models, there are no simple ways to reduce the computational effort for most applications in molecular simulation. We have no information about the existence of analytical or even hybrid methods capable to produce self-consistent closed-form solutions in cases where the interaction potential varies over time.

Our first attempt to simulate chemical reactions employed fractional derivatives to describe the evolution of a free radical reaction [9]. Nevertheless, fractional derivatives do not seem to be a suitable approach for nonlinear scattering processes.

However, after solving a particular version of the Klein-Gordon equation and finding some encouraging results in Nuclear Physics [10], we worked with some factorizations of this model, in order to obtain new analytical solutions. It occurs that some factorizations of the Klein-Gordon equation may produce a system of

first-order PDEs which is more general than the Dirac equations. The most general first-order system of PDEs obtainable via factorization of the Klein-Gordon model is the bi-quaternion Lanczos equation [11] [12] [13] [14]. This equation allows coupling the electronic cloud and the nucleus of a given atom in a unique structure, which can be describable by a single wave function. This characteristic reduces significantly the number of basic functions necessary to describe the chemical system. Each function represents an entire atom.

This work presents a new scalar quantum model based on an exact factorization for Klein-Gordon and Schrödinger-type equations. The new model differs from the standard ones in a fundamental way: it consists in a self-consistent nonlinear PDE whose dependent variable is the zeroth component of the Maxwell vector potential ( $A^0 = V$ ).

In order to eliminate the wave function from a given quantum model, a straightforward procedure based on Bäcklund transformations allows reformulating the target equation in such a way that a nonlinear one emerges. In the next section, it will be shown that some scalar quantum models can be obtained when a Bäcklund transformation is applied over a nonlinear model expressed only in terms of the interaction potential.

## 2. The Lorentz Force as a “Hydrodynamic” Model

When one choose the Lorentz gauge by imposing that the Maxwell vector potential obeys a differential constraint given by a continuity equation, namely

$$\frac{\partial A^0}{\partial t} + \frac{\partial A^1}{\partial x} + \frac{\partial A^2}{\partial y} + \frac{\partial A^3}{\partial z} = 0, \quad (2.1)$$

it is implicitly assumed that the gauge potential interacting with the molecules of the reactants behaves essentially as a compressible fluid. Hence, (2.1) represents a conservation law for a dynamic equation based on the Lorentz force:

$$m \frac{\partial v}{\partial t} = q(E + v \times B), \quad (2.2)$$

where  $m$  and  $q$  are, respectively, the mass and the charge of the electron,  $v$  stands for the electron velocity vector,  $E$  represents the electric field and  $B$  the magnetic induction. This equation can be writing in terms of the Maxwell vector potential as

$$m \frac{\partial v}{\partial t} = q \left( -\frac{\partial A^i}{\partial t} - \nabla \chi - v \times \nabla \times A^i \right). \quad (2.3)$$

Here  $A^i$  is the Maxwell vector potential and  $\chi$  represents a gauge potential. This system of partial differential equations implicitly states that the photon field interacts with the electronic clouds in such a way that Equations (2.1) and (2.2) can be regarded, respectively, as a continuity equation and a hydrodynamic model. This apparently naive analogy comes directly from a rigorous formalism, where dynamic equations arise from operator identities. These identities are commutation relations remaining valid even when dynamic equations and con-

servation laws break down.

## 2.1. The Maxwell Potential and the “Position” Photon Field

Since conservation laws come from a commutation relation between the time derivative and the divergent operator, namely

$$\left[ \frac{\partial}{\partial t}, \nabla \cdot \right] = 0. \quad (2.4)$$

Then there exists a field  $X$  defined by

$$\frac{\partial X}{\partial t} = A^i \quad (2.5)$$

and

$$\nabla \cdot X = -A^0, \quad (2.6)$$

reducing the Lorentz gauge to the following identity:

$$\left[ \frac{\partial}{\partial t}, \nabla \cdot \right] X \equiv 0. \quad (2.7)$$

Thus, Equations (2.4) and (2.5) represent solvability conditions for (2.1). The vector field  $X$  and the wave function play analogous roles in different areas of Physics. The field  $X$  is as a boson “position” vector whose diffuse character justifies the probabilistic approach of the traditional quantum mechanics. Moreover, it allows interpreting the minimal coupling as a natural consequence of the interplay between two velocity fields. The total momentum is defined as

$$p = mv + qA^i. \quad (2.8)$$

In this equation, the first term stands for the fermion contribution to the total momentum, while the second one is the respective boson counterpart. Roughly speaking, an electron is a vortex structure in a photon flow, so the electronic cloud has a structure whose qualitative features resembles a Kolmogorov cascade.

## 2.2. The Schrödinger Postulates as Solvability Conditions

The variables momentum and energy are defined in terms of the wave function as

$$p = -i\nabla\Psi, \quad (2.9)$$

and

$$E = i\frac{\partial\Psi}{\partial t}. \quad (2.10)$$

These definitions may be considered as a set of integrability conditions for the following partial differential equation:

$$\frac{\partial p}{\partial t} = -\nabla E. \quad (2.11)$$

In a sense, this equation constitutes a version of the second Hamilton’s equa-

tion. Notice that  $p$  is the gradient of a given scalar field and  $E$  is a time derivative of the same field. As in the former case, since the time derivative and the gradient operator commute, the definitions (2.8) and (2.9) are identically satisfied.

After this relatively long digression we are in position to find a possible structure for the interaction term in a scalar quantum model. Once the Maxwell potential is a photon velocity field, it seems reasonable to infer that both kinetic and potential energy can be expressed as quadratic forms. Suppose that a linear operator maps the potential into the wave function. Therefore, the equation written in terms of the potential function must present the same linear part of the original quantum model (Schrödinger or Klein-Gordon). In order to obtain a differential operator mapping the potential into the wave function it is convenient to find a Bäcklund transformation between some self-consistent equation and the original scalar quantum model.

### 2.3. Bäcklund Transformations as Mappings between PDEs

In order to eliminate the wave function from the Schrödinger equation, let us suppose that the potential function obeys the following quasi-linear second order model:

$$-\frac{1}{2} \frac{\partial^2 V}{\partial x^2} + \frac{1}{2} V^2 = i \frac{\partial V}{\partial t} \quad (2.12)$$

This model can suffer a reduction of order via Bäcklund transformations, generating a set of two auxiliary equations:

$$\frac{\partial V}{\partial x} = \varphi \quad (2.13)$$

and

$$i \frac{\partial V}{\partial t} = -\frac{1}{2} \frac{\partial \varphi}{\partial x} + \frac{1}{2} V^2 \quad (2.14)$$

In fact, (2.12) is obtained by replacing (2.13) in (2.14). Imposing the consistency between the definitions of the cross derivatives, it yields

$$i \frac{\partial^2 V}{\partial x \partial t} = \frac{\partial}{\partial x} \left( -\frac{1}{2} \frac{\partial \varphi}{\partial x} + \frac{1}{2} V^2 \right) = i \frac{\partial}{\partial t} (\varphi) \quad (2.15)$$

Hence, the following second order PDE for the wave function arises from this integrability condition:

$$-\frac{1}{2} \frac{\partial^2 \varphi}{\partial x^2} + V \frac{\partial \varphi}{\partial x} = i \frac{\partial \varphi}{\partial t} \quad (2.16)$$

Finally, replacing (2.13) in (2.16), the one dimensional time dependent Schrödinger equation is obtained:

$$-\frac{1}{2} \frac{\partial^2 \varphi}{\partial x^2} + V \varphi = i \frac{\partial \varphi}{\partial t} \quad (2.17)$$

In this Equation (expressed in atomic units) the parameters  $m$  and  $\hbar$  are absent, because  $m = \hbar = 1$ .

This process can be readily applied to the corresponding two dimensional Schrödinger equation. In this case, the starting point is the following two dimensional nonlinear model:

$$-\frac{1}{2}\left(\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2}\right) + \frac{1}{2}V^2 = i\frac{\partial V}{\partial t} \quad (2.18)$$

The corresponding auxiliary system becomes

$$\frac{\partial V}{\partial x} + i\frac{\partial V}{\partial y} = \varphi \quad (2.19)$$

and

$$i\frac{\partial V}{\partial t} = -\frac{1}{2}\left(\frac{\partial \varphi}{\partial x} - i\frac{\partial \varphi}{\partial y}\right) + \frac{1}{2}V^2. \quad (2.20)$$

In this case the linear differential operator which maps the potential into the wave function is defined by

$$L = \frac{\partial}{\partial x} + i\frac{\partial}{\partial y} \quad (2.21)$$

Since the time derivative commutes with operator  $L$ , it becomes possible to obtain the two dimensional Schrödinger equation after applying  $L$  over (2.21). Differentiating (2.19) respect to time, substituting in (2.20) and subtracting the resulting equations, it yields

$$i\frac{\partial \varphi}{\partial t} = -\frac{1}{2}LM\varphi + V\varphi. \quad (2.22)$$

In this equation,  $M$  represents the complex conjugate of  $L$ :

$$M = \frac{\partial}{\partial x} - i\frac{\partial}{\partial y}. \quad (2.23)$$

Hence,  $LM$  is the two dimensional Laplacian operator.

Notice that operators  $L$  and  $M$  contain only spatial derivatives. Thus, the mapping  $\varphi = LV$  is identical for the Schrödinger and Klein-Gordon equations. In other words, the Klein-Gordon equation arises by applying the same differential operator over the nonlinear model given by

$$\frac{\partial^2 V}{\partial t^2} - \frac{\partial^2 V}{\partial x^2} - \frac{\partial^2 V}{\partial y^2} = -\frac{1}{2}V^2 - mV. \quad (2.24)$$

In practice, since the mapping between the potential and the corresponding wave function does not specify the scalar quantum model employed, it becomes possible to choose a differential constraint to specify the particular physical scenario to simulate. Since our focus consists in describing the rearranging of the electronic cloud during a chemical reaction, it is possible to find a suitable differential constraint in electromagnetic theory: the Gauss law.

### 3. Analytical Solutions

The self-consistent potential is obtained by solving a steady form of the two di-

mensional Gauss law in complex variables. The exact solution obtained can be generalized in order to generate closed-form ones for the relativistic version of the model.

### Solving the Two Dimensional Nonlinear Gauss Law

It is possible to solve the Gauss law, given by

$$\frac{\partial^2 V}{\partial t^2} - \nabla^2 V = -\rho \tag{3.1}$$

using complex variables for time independent interaction potentials. This model reduces to the following equation:

$$\nabla^2 V = \rho = LVMV. \tag{3.2}$$

Once  $LM$  is the Laplacian operator, this equation can be written in the form  $LMV = (LV)(MV)$ , where  $L$  and  $M$  are respectively defined by (2.21) and (2.23). These operators are expressed in terms of the complex variables  $r = x + iy$  and  $s = x - iy$  as

$$L = \frac{\partial}{\partial x} + i \frac{\partial}{\partial y} = 2 \frac{\partial}{\partial s} \tag{3.3}$$

and

$$M = \frac{\partial}{\partial x} - i \frac{\partial}{\partial y} = 2 \frac{\partial}{\partial r}. \tag{3.4}$$

Thus, Equation (3.2) assumes the form

$$\frac{\partial^2 V}{\partial r \partial s} = \frac{\partial V}{\partial r} \frac{\partial V}{\partial s}. \tag{3.5}$$

It is possible to solve this equation directly by integration. Dividing by  $\frac{\partial V}{\partial s}$  and integrating in  $r$ , it yields

$$\ln \left( \frac{\partial V}{\partial s} \right) = V + \ln(f'(s)), \tag{3.6}$$

Here  $f(s)$  is an arbitrary function of  $s$ . This first-order partial differential equation can be promptly solved for  $V$ . Since

$$\frac{\partial V}{\partial s} = f'(s)e^V, \tag{3.7}$$

the potential function is obtained by multiplying both sides by  $e^{-V}$  and integrating in  $s$ :

$$-e^{-V} = f(s) + g(r). \tag{3.8}$$

Hence,

$$V = -\ln(a(r) + b(s)), \tag{3.9}$$

where  $a(r)$  and  $b(s)$  are arbitrary functions of its arguments. A natural extension of this solution to four dimensions naturally arises by defining a new set of va-

riables, namely

$$p = z + t \tag{3.10}$$

and

$$q = z - t. \tag{3.11}$$

Therefore, an exact four-dimensional solution is obtained:

$$V = -\ln(a(r, p) + b(s, p)). \tag{3.12}$$

Naturally, the former result could be generalized using Lie symmetries admitted by Equation (3.5). However, as will be showed in the next section, this sub-space solution yet satisfies a wide class of initial states and boundary conditions.

### 4. A Bi-Quaternion Model for the Potential

The bi-quaternion quantum model conceived by C. Lanczos in 1929 [11] [12] [13] [14] was initially ignored due to the rapid acceptance of the Dirac equations, which is widely recognized as the most important factorization of the Klein-Gordon equation. However, there are some interesting features in complex quaternion formulations. These features allow interpreting the scattering process as a boson gas flow. This point of view furnishes a more intuitive approach to Quantum Field Theory and provides a new method for finding self-consistent scattering potentials.

This section presents a new quantum model based on a simplified version of the Lanczos bi-quaternion formulation, which constitutes a new reduction of order for Klein-Gordon type equations. Such a factorization produces a set of first-order nonlinear PDEs containing the four vector Maxwell potential.

#### 4.1. Mapping Four Vectors into Spinors via Bi-Quaternion Operators

In previous sections, it was demonstrated that the operators  $L$  and its conjugate, namely  $M$  map interaction potentials into scalar wave functions, by converting the nonlinear partial differential equation given by

$$-\frac{1}{2}\left(\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2}\right) + \frac{1}{2}V^2 = i\frac{\partial V}{\partial t} \tag{4.1}$$

into the corresponding two-dimensional Schrodinger model

$$-\frac{1}{2}\left(\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2}\right) + V\varphi = i\frac{\partial \varphi}{\partial t}. \tag{4.2}$$

This mapping is identically satisfied by  $LV = \varphi$ . Since  $LM$  is the two-dimensional Laplacian operator, it is possible to generalize the scalar model by reformulating it in quaternion variables. In this four dimensional model,  $LM$  represents the D'Alembertian operator. In quaternion variables, the four vector  $\varphi^\mu = LA^\mu$  is given by

$$(\partial, i\nabla)(A^0, A) = \left(\frac{\partial A^0}{\partial t} - i\nabla \cdot A, \frac{\partial A}{\partial t} + i\nabla A^0 + i\nabla \times A\right). \tag{4.3}$$



Hence, the corresponding complex conjugate  $MA^\mu$  results

$$(\partial, -i\nabla)(A^0, A) = \left( \frac{\partial A^0}{\partial t} + i\nabla \cdot A, \frac{\partial A}{\partial t} - i\nabla A^0 - i\nabla \times A \right). \tag{4.4}$$

In these equations,  $A$  stands for the three-dimensional vector part of  $A^\mu$ , so the standard quaternion notation was adopted. Once the D'Alembertian operator is factorized as

$$\frac{\partial^2}{\partial t^2} - \nabla^2 = (\partial, i\nabla)(\partial, -i\nabla) = LM, \tag{4.5}$$

the set of four equations representing Gauss and Ampere's laws, namely

$$\frac{\partial^2 A^\mu}{\partial t^2} - \nabla^2 A^\mu = -j \tag{4.6}$$

can be recast as

$$LMA^\mu = -(LA^\mu)(MA^\mu). \tag{4.7}$$

In this equation, the right-hand side denotes the quaternion product between the four vectors  $\varphi^\mu = LA^\mu$  and  $\bar{\varphi}^\mu = MA^\mu$ :

$$(\varphi^0, \varphi)(\bar{\varphi}^0, \bar{\varphi}) = (\varphi^0 \bar{\varphi}^0 - \varphi \cdot \bar{\varphi}, \varphi^0 \bar{\varphi} + \bar{\varphi}^0 \varphi + \varphi \times \bar{\varphi}) \tag{4.8}$$

Here  $\varphi^\mu$  and  $\bar{\varphi}^\mu$  represents the four vector wave function and its conjugate bi-quaternion. Therefore, Equation (2.8) can also be express as a first-order system of nonlinear PDEs in these fields. Since  $L$  and  $M$  commute,

$$MLA^\mu = -(LA^\mu)(MA^\mu). \tag{4.9}$$

Thus, Equation (4.9) is written in the form

$$M(\varphi^0, \varphi) = -(\varphi^0, \varphi)(\bar{\varphi}^0, \bar{\varphi}), \tag{4.10}$$

or

$$L(\bar{\varphi}^0, \bar{\varphi}) = -(\varphi^0, \varphi)(\bar{\varphi}^0, \bar{\varphi}), \tag{4.11}$$

which corresponds to the original form of (4.9). Here the right hand side of both equations represents the quaternion definition of the current  $j$  appearing in Gauss and Ampere's laws.

### 4.2. The Influence of Gauge Potentials in the Interaction between Radiation and Matter

The properties of the operators  $L$  and  $M$  allows obtaining an explicit solution for the scalar self-consistent potential  $V = A^0$ . Once

$$\varphi = LV, \tag{4.12}$$

the Gauss law can be written as

$$LMV = -\varphi \bar{\varphi}. \tag{4.13}$$

However,

$$MV = \bar{\varphi}, \tag{4.14}$$

so Equation (4.14) can be express as

$$L\bar{\varphi} = -\varphi\bar{\varphi}. \tag{4.15}$$

Hence,

$$\varphi = -\frac{L\bar{\varphi}}{\bar{\varphi}}. \tag{4.16}$$

Since  $L$  is a first-order linear operator with constant coefficients,

$$\varphi = -L(\ln \bar{\varphi}) \tag{4.17}$$

Replacing (4.12) in the left hand side of (4.17), it yields

$$LV = -L(\ln \bar{\varphi}). \tag{4.18}$$

Therefore,

$$V = -\ln \bar{\varphi} + l \quad (Ll = 0). \tag{4.19}$$

Since  $L$  and  $M$  commute, Equation (4.13) can assume the form

$$MLV = -\varphi\bar{\varphi} \tag{4.20}$$

or

$$M\varphi = -\varphi\bar{\varphi}. \tag{4.21}$$

Thus,

$$\bar{\varphi} = -\frac{M\varphi}{\varphi} = -M(\ln \varphi). \tag{4.22}$$

Using (4.14), it results

$$MV = -M(\ln \varphi). \tag{4.23}$$

Hence,

$$V = -\ln \varphi + m \quad (Mm = 0). \tag{4.24}$$

In Equations (4.19) and (4.24), the functions  $l$  and  $m$  are gauge fields specifying the radiation interacting with the scattering medium. It occurs because these functions belong to the null space of the Laplacian operator. In other words, since  $LM = ML$  is the Laplacian operator and  $Ll = Mm = 0$ , then  $MLl = LMm = 0$ . Solving, (4.24) for the wave function and (4.9) for its complex conjugate, it yields

$$\varphi = e^{m-V} \quad (Mm = 0). \tag{4.25}$$

and

$$\bar{\varphi} = e^{l-V} \quad (Ll = 0). \tag{4.26}$$

Before interpreting these results, it becomes convenient to employ (4.12) and (4.14) to eliminate the wave function from this system of equations:

$$LV = e^{m-V} \tag{4.27}$$

and

$$MV = e^{l-V}. \tag{4.28}$$

But  $L$  and  $M$  can be written in terms of complex variables:

$$L = \frac{\partial}{\partial x} + i \frac{\partial}{\partial y} = 2 \frac{\partial}{\partial s} (s = x - iy) \tag{4.29}$$

and

$$M = \frac{\partial}{\partial x} - i \frac{\partial}{\partial y} = 2 \frac{\partial}{\partial r} (r = x + iy). \tag{4.30}$$

Therefore, Equations (4.27) and (4.28) can be expressed, respectively, as

$$2 \frac{\partial}{\partial s} V = e^{m-v} \tag{4.31}$$

and

$$2 \frac{\partial}{\partial r} V = e^{l-v}. \tag{4.32}$$

Rearranging terms, it yields

$$e^v \frac{\partial}{\partial s} V = \frac{1}{2} e^m \tag{4.33}$$

and

$$e^v \frac{\partial}{\partial r} V = \frac{1}{2} e^l. \tag{4.34}$$

Since  $Ll = Mm = 0$ ,  $l$  is an arbitrary function of  $r$  and  $t$ , while  $m$  is another arbitrary function of  $s$  and  $t$ . Hence, after integrating (4.33) respect to  $s$ , it results

$$e^v = \frac{1}{2} \int e^{m(s,t)} ds + a(r, t). \tag{4.35}$$

Analogously, integrating (4.34) respect to  $r$ , an equivalent definition for  $V$  arises:

$$e^v = \frac{1}{2} \int e^{l(r,t)} dr + b(s, t). \tag{4.36}$$

In these equations,  $a(r, t)$  and  $b(r, t)$  are arbitrary functions of its corresponding arguments. Once both definitions for the potential must be identical,

$$\frac{1}{2} \int e^{m(s,t)} ds = b(s, t). \tag{4.37}$$

and

$$\frac{1}{2} \int e^{l(r,t)} dr = a(r, t). \tag{4.38}$$

Finally, the general solution of the Gauss law for the potential function,

$$V = \ln(a(r, t) + b(s, t)), \tag{4.39}$$

emerges as a generalization of the scalar solution (3.12). Thus the two dimensional formulation can be employed to generate preliminary results.

The corresponding wave function is readily obtain from (4.25):

$$\varphi = e^{m - \ln(a(r,t) + b(s,t))}. \tag{4.40}$$

But  $m(s, t)$  can be written in terms of  $b(s, t)$  using (4.37):

$$m = \ln \left( 2 \frac{\partial b}{\partial s} \right). \quad (4.41)$$

Therefore,

$$\varphi = \frac{2}{a+b} \frac{\partial b}{\partial s}. \quad (4.42)$$

Similarly,

$$\bar{\varphi} = \frac{2}{a+b} \frac{\partial a}{\partial r}. \quad (4.43)$$

## 5. Results and Discussion

In this section, the analytical solutions given by Equations (3.9) and (3.12) are employed to simulate two basic scenarios in Quantum Chemistry. It is worth mentioning that the scale of the graphs presented is in Ångström.

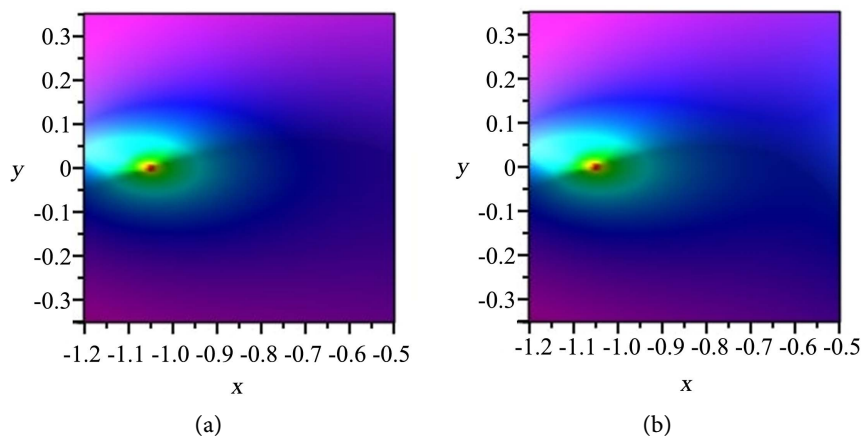
The first describes the process in which a typical ionic bonding arises between Potassium and Fluorine. **Figure 1(a)** show a Potassium atom, whose electron cloud suffers a slight shift towards the right direction. The cloud is migrating towards the Fluorine atom, which was intentionally not shown in both figures. This was done in order to emphasize the fact that the rearranging of the electron cloud occurs faster than the migration of the nuclei, which is consistent with the Born-Oppenheimer approximation. The electron cloud of the Fluorine atom begins to appear only in **Figure 1(b)**.

In **Figure 1(b)** the Fluorine atom finally appears. Although the Fluorine nucleus suffers attraction by the Potassium cloud, it slowly moves due to its relatively large mass. Notice that the cloud is distributed between the atoms in such a way that produces an ionic bond electron configuration.

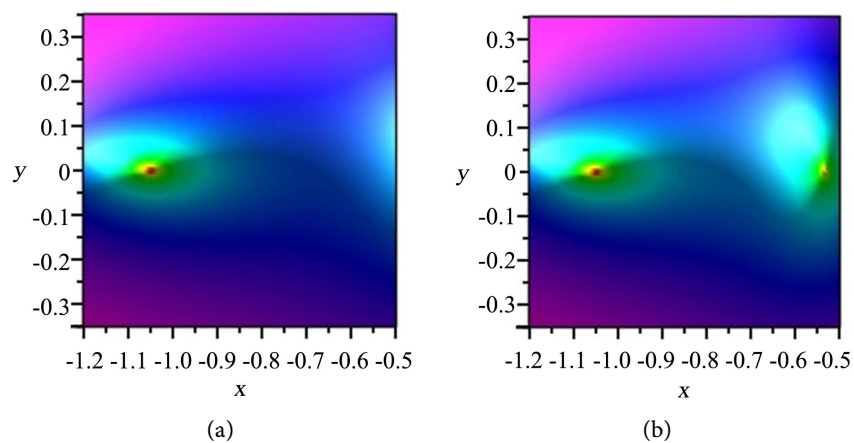
The second scenario illustrates the stability of aromatic rings. Two isolated chlorine atoms begin to attack the Hydrogen ones belonging to a benzene molecule as shown in **Figure 2(a)**. These Chlorine atoms are initially positioned in order to induce an interaction. Despite the apparently favorable attack position, the reaction does not occur. Instead, the electron cloud is attracted to the carbon atoms of the benzene ring. This electrophilic behavior is noticed by the intense blue region arising in **Figure 2(b)**.

The second scenario illustrates the stability of aromatic rings. Two isolated chlorine atoms begin to attack the Hydrogen ones belonging to a benzene molecule as shown in **Figure 3**.

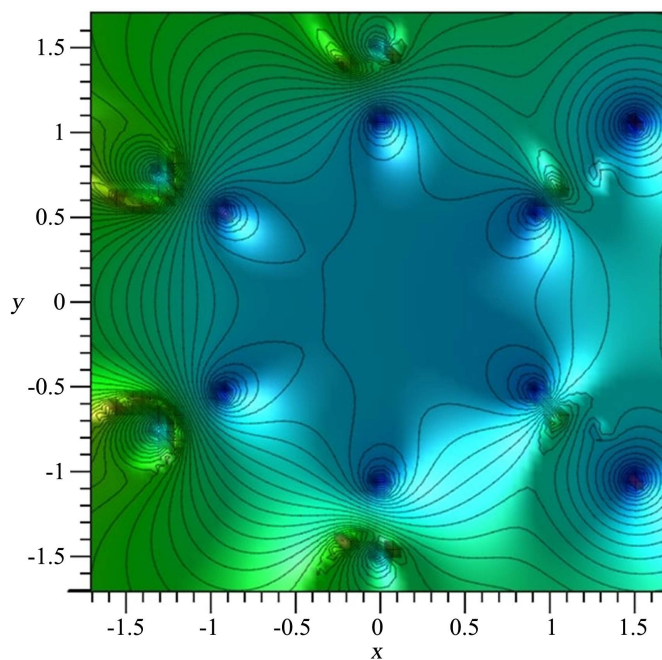
These Chlorine atoms are initially positioned in order to induce an interaction. Despite the apparently favorable attack position, the reaction does not occur. Instead, the electron cloud is attracted to the carbon atoms of the benzene ring. This electrophilic behavior is noticed by the intense blue region arising in **Figure 4**. In addition, we can see in **Figure 5** the Chlorine atoms attracting each other.



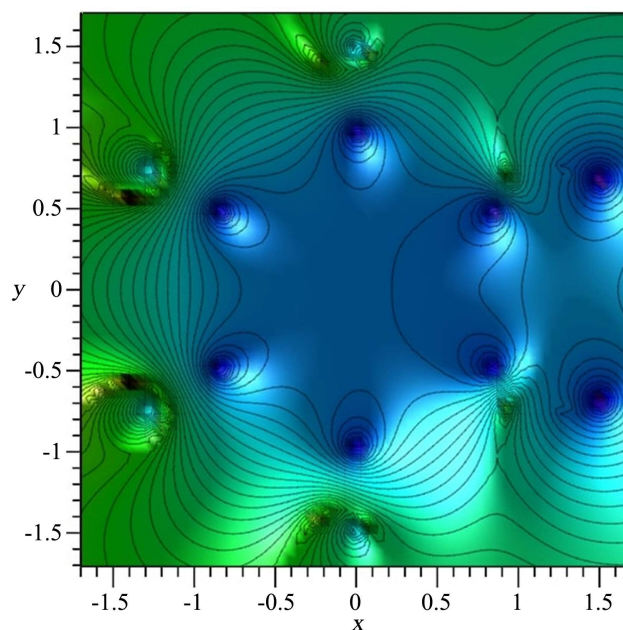
**Figure 1.** (a) and (b): electronic cloud migrating from K to F.



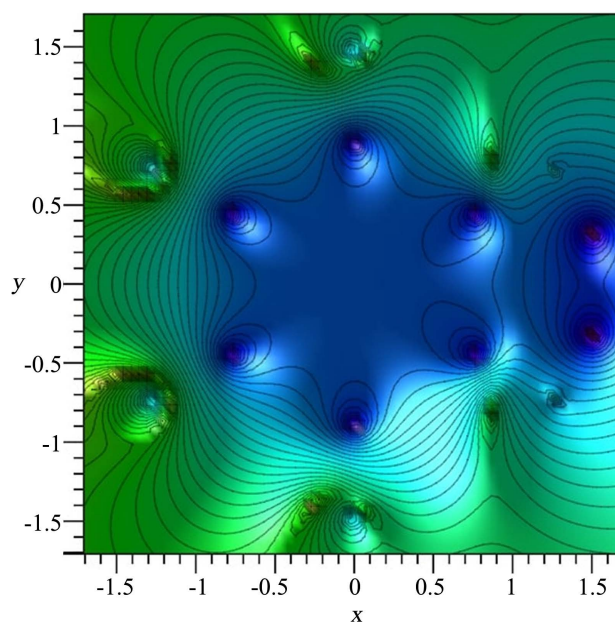
**Figure 2.** (a) and (b): consolidation of the ionic bond K-F.



**Figure 3.** Chlorine atoms positioned to attack a benzene ring.



**Figure 4.** Chlorine atoms attracting each other.



**Figure 5.** Chlorine atoms producing a covalent bond.

It is important to point out that the potential function describing atoms and molecules are approximate by truncated Laurent series. This representation demands a small computational effort to obtain the analytical solutions. The average time processing required to simulate a typical chemical reaction is about 3 seconds per atom (Macbook pro 2017, 16 GB RAM, using Maple).

## 6. Conclusions

The quantum model presented, although scalar, can be indirectly employed to

infer some fermion issues in the chemical scenarios. It occurs because it becomes possible to identify regions presenting high vorticity in the boson field represented by the potential function.

This analogy with fluid mechanics is not incidental. Notice that the photon field reveals much more about the molecular structure than the corresponding electron field because of the wide range of the boson action. In other words, the potential function allows showing some nonlocal effects that the fermion counterpart of the quantum model does not necessarily exhibit.

There are several other advantages of using quantum models written exclusively in terms of the potential function, in order to simulate chemical reactions:

1) The number of functions required to represent molecular systems is drastically reduced—typically one function per atom, while wave functions demand one function per electron. Eventually, some organic chains may be represented as truncated Laurent series containing few terms. In some cases, one function in complex variables is capable to approximate the potential of an entire organic chain or even a polymer.

2) The maps depicting the level curves of the total potential are considerably easier to interpret than the ones generated by total wave functions.

3) The formulation avoids some practical difficulties associated with the initial methods. As a result, the computational codes produced are small and easy to deurate.

4) The prescription of the initial state of the system becomes a simple task since all atoms involved present essentially the same shape, namely, the classical Lennard-Jones one.

5) For educational purposes, there exist exact solutions written in terms of the Weierstrass P function, whose behavior explains some interesting features of the so-called “quantum chaos” in a deterministic way.

6) Equation (2.1) admits solutions obtained through certain nonlinear combinations of previous exact ones. As a nontrivial consequence, it becomes possible to investigate whether two compounds react with each other.

7) The last advantage has an interesting application in catalysis. It occurs that if  $a$  and  $b$  are exact solutions of Equation (2.1), a new solution can be defined by  $V = a + b + h$ , where  $h$  is a particular solution of the corresponding linear model, namely

$$\frac{\partial^2 h}{\partial r \partial s} = 0 \quad (6.1)$$

This is the Laplace equation written in complex variables, so the solution  $h$  is a particular harmonic function that accounts for the gauge potential associated with the radiation that must be added to the compounds  $a$  and  $b$  in order to deflagrate the reactive process. It is easy to show that when  $V = a + b + h$  is replaced in Equation (2.18), a new solution emerges:

$$V = \sqrt{a^2 + b^2} . \quad (6.2)$$



This function stands for a final bound containing less energy than the sum of the energies of the isolated original reactants. Hence, even adding the gauge field  $h$  in order to promote the reaction between the compounds represented by the potentials  $a$  and  $b$ , the final result is a bound state that is less energetic than the initial configuration of the system. In other words, even after adding the activation energy, represented by the field  $h$ , the system evolves and reaches a final state described by Equation (6.2).

Bearing in mind all the practical advantages of using quantum models expressed in terms of the potential function, we step forward by formulating new vector and tensor models, in order to improve and generalize the results obtained. In future works, we intend to implement new software based on the bi-quaternion formulation, which allows simulating the time evolution of the electron cloud and the subtle corresponding perturbations in the nuclei structure. From this coupling between nuclei and electronic clouds, we expect that new relevant information about the spin-orbital interaction will finally emerge in a simple way. Considering the encouraging preliminary results yet obtained, we hope that some *a priori* unintuitive features of Quantum Field Theory will also elucidate after being analyzed under this point of view.

## Conflicts of Interest

The authors declare no conflicts of interest.

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