BEYOND QUANTUM NONLOCALITY: CHEMICAL BONDING FIELD

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Abstract: *New concept of quantum chemistry, namely chemical bonding field □, is introduced in the context of Bohmian treatment of Schrödinger equation with u(1) nonlocal gauge transformation of the de Broglie wavefunction.*
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1. INTRODUCTION

In current scientifically quests the international community arrives at the *mysteries Decalogue* that has to be unfolded by the present or next generations of knowledge or designing the main lines towards which the human ideatic efforts should be concentrated in order to equilibrate the historic questions with the advances in observing and modifying reality. Eventually they are (see also the inaugural essay of this Journal issue) [1]:

- What was before the Big-Bang?
- How the living nature has emerged?
- What are the relationships between the genes and embryos?
- We are alone in Universe?
- We are living a quantum world?
- What is time?
- How the conscience is formed?
- From where comes the ideas?
- What is the specific difference of man among other creatures?
- How the end of the Word will look like?

Observe that the half of these inquires belongs to Physics, three to Biology, and the other two to the so called Neuro-Sciences; where is Chemistry? An honest answer would place Chemistry at the edges between Physical and Biological and between Biological and Neuro Sciences since it really accounts on the quantification of bonds, either among various substances or inside and outside of the living organisms.

Therefore, the inner nature of the Chemistry itself seems to resume at bonding: the structure stability, the reactivity propensity.

Yet, the Chemistry has to provide a viable answer to this major problem;

- What the Chemical Bond features?

This question is raised by the somehow ambiguous nature of chemical bond that equally admit a static and a dynamic picture when treating an isolated or in interaction electronic system, respectively. In other words, although quantum mechanics widely provided the necessary tools for properly describing the atomic, molecular and of their interactions, a specific measure of chemical bond and bonding is still missing.

The present work likes for the first time to introduce the possible assessment of the chemical bond while encompassing both structure and reactivity information within the quantum mechanical Bohmian context combined with simple unitary U(1) gauge transformation; it leads with a simple yet meaningful quantity easy to handle and use in both macro-and microscopic resolution hoping in further application of it in all branches of physical-chemistry; it may eventually be generalized for better characterizing the environmental interactions (bio-chemo, neuro-chemo, eco-chemo) and to finally reach the quantum-classical bridge between the hidden and observed reality.

2. BASIC DE BROGLIE-BOHM-SCHRÖDINGER FORMALISM

The starting point resides in considering the de Broglie-Bohm electronic wavefunction [2],

$$\Psi_{BB}(x,t) = R(x,t) \ \exp\left(i \frac{S(x,t)}{\hbar} \right), \qquad (1)$$

with the *R*-amplitude and *S*-phase factors given respectively as:

$$R(x,t) = \sqrt{\Psi(x,t)^2} = \rho^{1/2}(x), \qquad (2a)$$

$$S(x,t) = px - Et = S_0 - Et, \qquad (2b)$$

in terms of electronic density ρ, momentum p, total energy E, and space-time (x,t) coordinates, without spin.

In these conditions, since one perfumes the wavefunction partial derivatives respecting space and time,

$$\frac{\partial^2 \Psi_{BB}}{\partial x^2} = \left[\frac{\partial^2 R}{\partial x^2} + 2\frac{i}{\hbar}\frac{\partial R}{\partial x}\frac{\partial S}{\partial x} + \frac{i}{\hbar}R\frac{\partial^2 S}{\partial x^2} - \frac{R}{\hbar^2}\left(\frac{\partial S}{\partial x}\right)^2 \right] \exp\left(\frac{i}{\hbar}S\right), \quad (3a)$$

$$\frac{\partial \Psi_{BB}}{\partial t} = \left[\frac{\partial R}{\partial t} + \frac{i}{\hbar}R\frac{\partial S}{\partial t} \right] \exp\left(\frac{i}{\hbar}S\right), \qquad (3b)$$

the conventional Schrödinger equation [3]

$$i\hbar \frac{\partial \Psi_{BB}}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi_{BB}}{\partial x^2} + V\Psi_{BB} \qquad (4)$$

takes the real and imaginary forms:

$$\frac{\partial R}{\partial t} = -\frac{1}{2m}\left[2\frac{\partial R}{\partial x}\frac{\partial S}{\partial x} + R\frac{\partial^2 S}{\partial x^2} \right], \qquad (5a)$$

$$-R\frac{\partial S}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 R}{\partial x^2} + \frac{R}{2m}\left(\frac{\partial S}{\partial x}\right)^2 + VR, \qquad (5b)$$

that can be further arranged as:

$$\frac{\partial R^2}{\partial t} + \frac{\partial}{\partial x}\left[\frac{R^2}{m}\frac{\partial S}{\partial x} \right] = 0, \qquad (6a)$$

$$\frac{\partial S}{\partial t} - \frac{\hbar^2}{2m}\frac{1}{R}\frac{\partial^2 R}{\partial x^2} + \frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2 + V = 0. \qquad (6b)$$

Worth noting that the first equation (6a) recovers in 3D coordinates the charge current (j) conservation law,

$$\frac{\partial \rho}{\partial t} + \Delta j = 0, \, j = \left(R^2/m \right)\overline{\Delta S}, \qquad (7a)$$

while the second equation (6b) in 3D,

$$\frac{\partial S}{\partial t} - \frac{\hbar^2}{2m}\frac{\nabla^2 R}{R} + \frac{1}{2m}(\nabla S)^2 + V = 0 \qquad (7b)$$

extends the basic Schrödinger equation (4) to include further quantum complexity. It may be clearly seen since recognizing that:

$$(\Delta S)^2 = p^2 \Rightarrow \frac{1}{2m}(\Delta S)^2 = \frac{p^2}{2m} = T; \frac{\partial S}{\partial t} = -E \qquad (8)$$

one gets from (7b) the total energy expression:

$$E = T + V + V_{qua} \qquad (9a)$$

in terms of newly appeared so called quantum (or Bohm) potential

$$V_{qua} = -\frac{\hbar^2}{2m}\frac{\Delta^2 R}{R}. \qquad (9b)$$

Exploring the consequences of the existence of the Bohm potential (9b) reveals most interesting features of the fundamental nature of electronic quantum behavior. We will survey some of them in what follows.

2.1 Limits of V_{qua}

From definition (9b) one can easily yield that the Bohm potential comprises both classical and infinitely manifested quantum characters:

$$V_{qua} = \begin{cases} \infty, & m \to 0, \text{ ...small quantum particles} \\ 0, & \frac{\hbar}{m} \to 0, \text{ ...classical particles and limit} \end{cases} \qquad (10)$$

2.2 The Case $V_{qua} = T$

If the whole particle kinetic energy is "created" from the quantum potential,

$$V_{qua} = T = E - V \qquad (11)$$

then the quantum potential (9b) resembles the stationary Schrödinger equation under the form:

$$-\frac{\hbar^2}{2m}\nabla^2 |\Psi_{BB}| = (E - V)|\Psi_{BB}| \qquad (12)$$

when considering from the first part of (2a) the equivalence $R = |\Psi_{BB}|$.

Note that while factorizing the wavefunction (1) on spatial and temporal contributions,

$$\Psi_{BB}(x,t) = \Psi_{BB0}(x)\exp\left(-\frac{E \cdot t}{\hbar} \right), \qquad (13a)$$

$$\Psi_{BB0}(x) = R_0(x)\ \exp\left(\frac{i}{\hbar}S_0 \right), \qquad (13b)$$

$$R_0^2 = \Psi_{BB0}^2(x) = \Psi_{BB}^2(x,t), \qquad (13c)$$

the equality (11) between its extreme parts holds when the spatial wave function domain is restricted to the real realm only, i.e.

$$\Psi_{BB0}(x) \in \Re \Rightarrow S_0 = 0 \Rightarrow p = 0 \Rightarrow T = 0 \Rightarrow E = V + V_{qua}. \quad (14)$$

Such situation is specific to electrons in their rest or s- or Y_{nl0}- states in atoms, encompassing therefore a complex quantum dynamical equilibrium. Such result reopens the issue of providing a quantum analytical base of the first Bohr postulate concerning the stationary states in bonded quantum systems.

2.3 The First Bohr Postulate Reloaded

We have to show the two ways of the equivalence between the total force acting upon a particle moving in a potential field and the time conservation of its total energy:

$$F = -\overline{\nabla}V_{tot}\left(= -\overline{\nabla}V_{qua} + \overline{\nabla}V\right) = m\ddot{x} \Leftrightarrow E = \frac{m}{2}\dot{x}^2 + V_{tot}(x(t)) = CT. \, IN \, TIME \quad (15)$$

The left-to-right proof is immediate and based on common analytical mechanics: if one differentiates both parts of a general total energy there is immediate that:

$$\frac{\partial E}{\partial t} = m\dot{x}\ddot{x} + \nabla V_{tot}\dot{x} = 0 \quad (16)$$

when the left side prescription of (15) applies.

Reciprocally, assuming the explicit time independence of total energy, we practically have that:

$$E = ct \Rightarrow \frac{\partial^2 S}{\partial t^2} = \frac{\partial}{\partial t}(-E) = 0; \quad (17a)$$

Now, implementing (17a) together with other space-time Bohm S-phase factor relationships,

$$\frac{\partial}{\partial t}\Delta S = \frac{\partial}{\partial t}p = \frac{\partial}{\partial t}m\dot{x} = m\ddot{x}, \quad (17b)$$

$$\frac{\nabla S}{m} = \frac{p}{m} = \frac{m\dot{x}}{m} = \dot{x} \quad (17c)$$

in the partial time-derivative operator applied on equation (7b),

$$\frac{\partial^2 S}{\partial t^2} + \frac{\partial V_{qua}}{\partial x}\frac{\partial x}{\partial t} + \frac{\nabla S}{m}\frac{\partial}{\partial t}\nabla S + \frac{\partial V}{\partial x}\frac{\partial x}{\partial t} = 0, \quad (18a)$$

there is immediate to obtain the left side expression of (15):

$$m\ddot{x} = F_{tot} = F_{clas} + F_{qua} = -\overline{\nabla}V - \overline{\nabla}V_{qua} \quad (18b)$$

This way, the stationarity Bohr postulate combine both classical and quantum characters in close agreement with the eigen- or observable states it beholds. Further consideration respecting the Bohr quantification in the Bohm context was elsewhere addressed [4].

2.4 Locality in Bonding Systems

When both $V_{qua}=T$ and spatial conservation of total energy $E=V+V_{qua}$ are assumed, the particle localization condition unfolds as:

$$0 = \frac{\partial E}{\partial x} = -\overline{\nabla}V - \overline{\nabla}V_{qua} = F_{clas} + F_{qua} = F_{tot} \quad (19)$$

leading with the idea that, experimentally, a particle is observed as corpuscle only when the cloassical force applied (aka the measurement apparatus) reaches through its range of action the negative of the quantum potential associate with the Schrödinger stationary (or eigen) state.

2.5 Nonlocality in Bonding Systems

Although manifestly in quantum stationarity and localization the quantum potential (9b) comprises the inherent nonlocality features as well. For instance, one could observe that the quantum field is independent of the intensity of measurement (the magnitude of *aR*) but dependent only on its form:

$$V_{qua} = -\frac{\hbar^2}{2m}\frac{\Delta^2(aR)}{(aR)} = -\frac{\hbar^2}{2m}\frac{\Delta^2 R}{R} \quad (20)$$

Moreover, since according with the basic properties of correct wavefunctions we have that while the entirely as well as the amplitude of de Broglie-Bohm wave-packet cancel at "infinitum",

$$\Psi_{BB}(x \to \infty) = 0; \, R(x \to \infty) = 0 \quad (21)$$

the quantum potential (20) do not vanish asymptotically, meaning that it does not behave locally, being distributed in a spatial-temporal manner assuring the nonlocal or non-separated or entangled interaction [5].

An immediate generalization for many-body systems may be as well furnished for the generalized Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}\Psi_{BB}(x_1,...,x_N,t) = \left[-\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 + V\right]\Psi_{BB}(x_1,...,x_N,t), \quad (22a)$$

with

$$\Psi_{BB}(x_1,...,x_N,t) = R(x_1,...,x_N,t) \, \exp\left(i\frac{S(x_1,...,x_N,t)}{\hbar}\right), \quad (22b)$$

while the *N*-body quantum potential becomes

$$V_{N-qua} = -\frac{\hbar^2}{2m}\frac{\nabla^2 R(x_1,...,x_N,t)}{R(x_1,...,x_N,t)}, \quad (22c)$$

Going to interpret the *N*-particles quantum field (22c) influence in nonlocality note that as it is not a decreasing function of distance the behavior of each particle may depend non-locally on the configuration of all others, no matter how far they may be.

In these conditions, the next conceptual issue rises:

- How to understand the existence of individual objects when non-local entanglement states are over entire Universe extended?

Such paradox may be fortunately solved out by means of the fact that not all systems are equally correlated; actually, analytical independence may be achieved by considering the total wave function (22b) as a factorized product of individual independent wave functions,

$$\Psi_{BB}(x_1,...,x_N,t) = \prod_{i=1}^{N} \Psi_{BBi}(x_i,t), \qquad (23a)$$

in which case the quantum potential (22c) rewrites as the sum of individual terms:

$$V_{N-qua} = \sum_{i=1}^{N} V_{i-qua} = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\frac{\nabla^2 R(x_i,t)}{R(x_i,t)}. \qquad (23b)$$

Now, the interactions between each *i*-subunit may be treated din traditional (observable) chemical way, while their inner quantum behavior is driven by non-local interactions. Nevertheless, despite the present consideration considerably enlarges the quantum mechanical concepts and power of interpretation for the causes of things and of their interactions, the concrete measure of chemical bonding is still missing from the Bohmian quantum mechanics–a matter that is to be in next introduced; it has to be related either with locality of electronic pairs as well as with the nonlocality in what delocalization of electrons is concerned. In other words the chemical bonding field may be seen as the critical reality that transforms the locality in nonlocality and vice-versa; in this sense, it would be considered as the major concept in springing life and observable objects in Universe!

3. INTRODUCING CHEMICAL BONDING FIELD

3.1 Schrödinger Equation for U(1) Wavefunction

Since the chemical bonding is carried by electrons only, one can see the basic de Broglie-Bohm wavefunction (1) as belonging to gauge U(1) group transformation:

$$\Psi_{U(1)}(x,t) = \Psi_{BB}(x,t)\exp\left(\frac{i}{\hbar}\frac{e}{c}\aleph(x,t)\right)$$

$$= R(x,t)\ \exp\left[\frac{i}{\hbar}\left(S(x,t)+\frac{e}{c}\aleph(x,t)\right)\right], e = \frac{e_0^2}{4\pi\varepsilon_0}, \quad (24)$$

where the *chemical field* □ should account through of variational principle (Schrödinger equation here) by the electronic bond, eventually being quantified by associate corpuscle.

As such, one employs the gauge wavefunction (24) to compute the actual Schrödinger partial derivative terms as:

$$\frac{\partial\Psi_{U(1)}}{\partial x} = \left[\frac{\partial R}{\partial x}+\frac{i}{\hbar}R\left(\frac{\partial S}{\partial x}+\frac{e}{c}\frac{\partial\aleph}{\partial x}\right)\right]\exp\left[\frac{i}{\hbar}\left(S+\frac{e}{c}\aleph\right)\right], \quad (25a)$$

$$\frac{\partial^2\Psi_{U(1)}}{\partial x^2} = \left\{\begin{array}{l}\frac{\partial^2 R}{\partial x^2}+2\frac{i}{\hbar}\frac{\partial R}{\partial x}\left(\frac{\partial S}{\partial x}+\frac{e}{c}\frac{\partial\aleph}{\partial x}\right)+\frac{i}{\hbar}R\left(\frac{\partial^2 S}{\partial x^2}+\frac{e}{c}\frac{\partial^2\aleph}{\partial x^2}\right) \\ -\frac{R}{\hbar^2}\left[\left(\frac{\partial S}{\partial x}\right)^2+\left(\frac{e}{c}\frac{\partial\aleph}{\partial x}\right)^2\right]-2\frac{e}{\hbar^2 c}R\frac{\partial S}{\partial x}\frac{\partial\aleph}{\partial x}\end{array}\right\}\exp\left[\frac{i}{\hbar}\left(S+\frac{e}{c}\aleph\right)\right], \quad (25b)$$

$$\frac{\partial\Psi_{U(1)}}{\partial t} = \left[\frac{\partial R}{\partial t}+\frac{i}{\hbar}R\left(\frac{\partial S}{\partial t}+\frac{e}{c}\frac{\partial\aleph}{\partial t}\right)\right]\exp\left[\frac{i}{\hbar}\left(S+\frac{e}{c}\aleph\right)\right], \quad (25c)$$

leading with the decomposition of the corresponding Schrödinger U(1) equation on the imaginary and real parts respectively:

$$-\frac{\partial R}{\partial t} = \frac{1}{m}\left(\frac{\partial R}{\partial x}\frac{\partial S}{\partial x}+\frac{R}{2}\frac{\partial^2 S}{\partial x^2}\right)+\frac{e}{mc}\left(\frac{\partial R}{\partial x}\frac{\partial\aleph}{\partial x}+\frac{R}{2}\frac{\partial^2\aleph}{\partial x^2}\right), \quad (26a)$$

$$-R\frac{\partial S}{\partial t}-R\frac{e}{c}\frac{\partial\aleph}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 R}{\partial x^2}+\frac{R}{2m}\left[\left(\frac{\partial S}{\partial x}\right)^2+\left(\frac{e}{c}\frac{\partial\aleph}{\partial x}\right)^2\right]+\frac{e}{mc}R\frac{\partial S}{\partial x}\frac{\partial\aleph}{\partial x}+VR, \quad (26b)$$

that can be further rearranged as:

$$-\frac{\partial R^2}{\partial t} = \frac{1}{m}\frac{\partial}{\partial x}\left(R^2\frac{\partial S}{\partial x}\right)+\frac{e}{mc}\frac{\partial}{\partial x}\left(R^2\frac{\partial\aleph}{\partial x}\right), \quad (27a)$$

$$-\left(\frac{\partial S}{\partial t}+\frac{e}{c}\frac{\partial\aleph}{\partial t}\right) = -\frac{\hbar^2}{2m}\frac{1}{R}\frac{\partial^2 R}{\partial x^2}+\frac{1}{2m}\left[\left(\frac{\partial S}{\partial x}\right)^2+\left(\frac{e}{c}\frac{\partial\aleph}{\partial x}\right)^2\right]+\frac{e}{mc}\frac{\partial S}{\partial x}\frac{\partial\aleph}{\partial x}+V. \quad (27b)$$

Equations (27) reveal some interesting features of the chemical bonding to be in next discussed.

3.2 Chemical Field Charge Current

The equation (27a) provides the conserving charge current with the form:

$$j_{U(1)} = \frac{R^2}{m}\left(\overline{\nabla S}+\frac{e}{c}\overline{\nabla\aleph}\right) = j_S + j_\aleph \qquad (28)$$

leaving with idea that additional current is responsible for the chemical field to be activated, namely:

$$j_\aleph = \frac{e}{mc}R^2\overline{\nabla\aleph} \qquad (29)$$

which vanishes when the *global gauge* condition is considered, i.e. when

$$\frac{\partial \aleph}{\partial x} = 0 \qquad (30)$$

Therefore, in order the chemical bonding be created the *local gauge* transformation should be used that is

$$\frac{\partial \aleph}{\partial x} \neq 0. \qquad (31)$$

In these conditions, the chemical field current (29) carries specific bonding particles that can be appropriately called as *bondons*, closely related with electrons, in fact with the those electrons involved in bonding, either as single, lone pair or delocalized, and having an oriented direction of moving, with an action depending on chemical field itself □.

3.3 Gauge Chemical Bonding Fields

Nevertheless, another important idea abstracted from above discussion is that going to search the chemical field □ no global gauge condition as (30) should be used. Worth noting as well that the presence of the chemical field do not change the Bohm quantum potential (9b) which is recovered untouched in (27b) thus preserving the entanglement of interaction. With his there follows that in order the de Broglie-Bohm-Schrödinger formalism and equations (6) to be invariant under gauge U(1) transformation (24) a couple of gauge conditions the chemical field has to fulfilled out of equations (27); they are respectively:

$$\frac{e}{mc}\frac{\partial}{\partial x}\left(R^2 \frac{\partial \aleph}{\partial x}\right) = 0, \qquad (32a)$$

$$\frac{e}{c}\frac{\partial \aleph}{\partial t} + \frac{1}{2m}\left(\frac{e}{c}\frac{\partial \aleph}{\partial x}\right)^2 + \frac{e}{mc}\frac{\partial S}{\partial x}\frac{\partial \aleph}{\partial x} = 0. \qquad (32b)$$

Now, the chemical field □ is found through combining its spatio-temporal information contained in equation (32). From condition (32a) is getting that:

$$\overline{\nabla \aleph} = -R\frac{\nabla^2 \aleph}{\nabla R \cdot \vec{j}}\vec{j}, \qquad (33)$$

where the vectorial feature of the chemical field gradient was emphasized on the direction of its associated charge current (29) fixed by the versor $\vec{j}$ ($j^2 = 1$). We will maintain such procedure whenever necessary for avoiding scalar to vector ratios and preserving the physical sense of the whole construction as well.

Next, the gradient (33) is replaced in (32b) to obtain a single equation for the chemical field:

$$\frac{e}{2mc}\frac{R^2}{(\nabla R)^2}\left(\nabla^2 \aleph\right)^2 - \frac{R}{m}\frac{\overline{\nabla S}\cdot\overline{\nabla S}}{\overline{\nabla R}\cdot\overline{\nabla S}}\left(\nabla^2 \aleph\right) + \frac{\partial \aleph}{\partial t} = 0 \qquad (34)$$

that can be further rewritten as:

$$2\frac{e}{mc}\frac{\rho^2}{(\nabla \rho)^2}\left(\nabla^2 \aleph\right)^2 - 2\frac{\rho\vec{v}\cdot\vec{j}}{\overline{\nabla \rho}\cdot\vec{j}}\left(\nabla^2 \aleph\right) + \frac{\partial \aleph}{\partial t} = 0 \qquad (35)$$

since calling the relations:

$$R = \rho^{1/2}; \overline{\Delta S} = \vec{p} \Rightarrow \begin{cases} \nabla R = \frac{1}{2}\frac{\nabla \rho}{\rho^{1/2}}; \quad (\nabla R)^2 = \frac{1}{4}\frac{(\nabla \rho)^2}{\rho} \\ \frac{\overline{\nabla S}\cdot\overline{\nabla S}}{\overline{\nabla R}\cdot\overline{\nabla S}} = \frac{2\rho^{1/2}\vec{p}\cdot\vec{j}}{\overline{\nabla \rho}\cdot\vec{j}} \end{cases} \qquad (36)$$

Equation (35) can be solved for the Laplacian of the chemical field with general solutions:

$$\left(\nabla^2 \aleph\right)_{1,2} = \frac{2\frac{\rho\vec{v}\cdot\vec{j}}{\overline{\nabla \rho}\cdot\vec{j}} \pm \sqrt{\frac{4\rho^2 v^2}{(\nabla \rho)^2} - 4\frac{2e}{mc}\frac{\rho^2}{(\nabla \rho)^2}\frac{\partial \aleph}{\partial t}}}{\frac{4e}{mc}\frac{\rho^2}{(\nabla \rho)^2}}. \qquad (37)$$

Equation (37), is a special propagation equation for the chemical field since it links the spatial Laplacian $\Delta^2 \aleph = \Delta \aleph$ with temporal evolution of the chemical field $(\partial \aleph / \partial t)^{1/2}$; however, it may be considerable be simplified if assuming the stationary chemical field, i.e. chemical field as not explicitly depend on time,

$$\frac{\partial \aleph}{\partial t} = 0, \qquad (38)$$

in agreement with the fact that once established the chemical bonding should be manifested stationary in order to preserve the stability of the structure it applies.

With condition (38) we may still have two solutions for the chemical field.

• One corresponds with the *homogeneous* chemical bonding field

$$\Delta \aleph = 0 \Rightarrow \aleph_h = \frac{mc}{e}v_{\vec{j}} \; X_{bond} \qquad (39)$$

with the constant determined such that the field (39) to be of the same nature as the Bohm phase action S in (24).

• The second solution of (37) looks like

$$\Delta \aleph = \frac{mc}{e}\frac{v.\Delta\rho}{\rho}. \qquad (40)$$

Finally, equation (40) may be integrated to primarily give:

$$\overline{\nabla \aleph} = \frac{mc}{e}\vec{v} \int_\infty^r \frac{\overline{\nabla \rho} \cdot \vec{j}}{\rho} dx = \frac{mc}{e}\vec{v} \left[\int_\infty^0 \frac{\overline{\nabla \rho} \cdot \vec{j}}{\rho} dx + \int_0^r \frac{\overline{\nabla \rho} \cdot \vec{j}}{\rho} dx \right] \quad (41)$$

that can be projected on *bondonic* current direction $\vec{j}$ and then further integrated as:

$$\aleph - \aleph_0 = \frac{mc}{e}v_{\vec{j}}X_{bond}\left(\int_\infty^0 \frac{\overline{\nabla \rho} \cdot \vec{j}}{\rho} dl\right) + \frac{mc}{e}v_{\vec{j}}\int_0^{x(t)}\left(\int_0^r \frac{\overline{\nabla \rho} \cdot \vec{j}}{\rho} dl\right)dr, \quad (42)$$

from where there is identified both the so called *manifested* chemical bond field:

$$\aleph_0 = \frac{mc}{e}v_{\vec{j}}X_{bond}\left(\int_0^\infty \frac{\overline{\nabla \rho} \cdot \vec{j}}{\rho} dl\right), \quad (43a)$$

for a given inter-nuclear distance X_{bond}, as well as the *delocalized* chemical bond field:

$$\aleph(x(t)) = \frac{mc}{e}v_{\vec{j}}\int_0^{x(t)}\int_0^r \frac{\overline{\nabla \rho} \cdot \vec{j}}{\rho} dr dl \quad (43b)$$

which is the most general stationary chemical bonding field without spin.

Worth commenting on the integrand of above chemical bonding fields, since it accounts for the entangled distance concerned; as such, the expression (43b) converges to (43a) when and meaning that the $x(t) \to \infty$ and $r \to X_{bond}$ meaning that the X_{bond} is (locally) manifested in the infinite bath of nonlocal (entangled) interactions. Relation (39) may be as well recovered from (43b) when the density gradient becomes $\Delta \rho \to \rho/X_{bond}$ and $x(t) \to r \to X_{bond}$ revealing that the electronic system is completely isolated and with a uniform charge distribution along bonding (no no-local interactions admitted).

Another interesting point regards the general density gradient dependency of the chemical field (43b), a feature that finely resembles two important results of quantum chemistry:

- The gradient expansion when chemical structure and bonding is described in the context of density functional theory [6];
- The Bader zero flux condition for defining the basins of bonding [7], that in the present case is represented by the zero chemical boning fields, viz.:

$$\aleph = 0 \Leftrightarrow \overline{\Delta \rho} \cdot \vec{j} = 0 \quad (44)$$

It is this last feature the decisive reason that the aleph function in gauge transformation (24) is correctly associated with chemical bonding!

3.4 Bondons: Chemical Elementary Particles of Bonding

Last issue addresses the range values of the chemical bonding field as well as its physical meaning. For the typical values enough observing that from the gauge U(1) transformation (24) that the chemical bonding field has to be in relation with the inverse order of the fine-structure constant:

$$\aleph_{bondon} \sim \frac{\hbar c}{e} \sim 137.03599976 \frac{Joule \times meter}{Coulomb}, \quad (45)$$

an enough small quantity, in quantum range, to be apparently neglected, however, with crucial role for chemical bonding where the energies involved are about orders of 10^{-19} Joules (electron-volts)! Nevertheless, for establishing the physical significance of the chemical bonding quanta field (45) one can proceed with the chain equivalences:

$$\langle \aleph \rangle \sim \frac{energy \times distance}{charge} \sim \frac{\left(charge \times \frac{potential}{difference}\right) \times distance}{charge} \sim \left(\frac{potential}{difference}\right) \times distance. \quad (46)$$

The combined phenomenology of the results (45) and (46) states that: the chemical bonding field caries *bondons* with unit quanta (45) along the distance of bonding within the potential gap of stability or by tunneling the potential barrier of encountered bonding attractors.

Alternatively, from the generic form (39) for the chemical field, if one replaces the velocity by the kinetic energy and making then use by Heisenberg relationship, viz.

$$v = \sqrt{\frac{2T}{m}} \sim \sqrt{\frac{2}{m}\frac{\hbar}{t}}, \quad (47a)$$

the space-chemical bonding field dependence is simply achieved as:

$$\aleph \sim \left(\frac{c\hbar}{e}\sqrt{\frac{2m}{\hbar t}}\right)X_{bond} \sim 4.28715 \cdot 10^{13}X_{bond} \quad (47b)$$

where we can assume various instantaneous times according with the studied phenomena. At one extreme, when the ration of the first Bohr radius ($a_0 = 0.52917.10^{-10} m$) to the speed velocity is assumed, $t \to t_0 = a_0/c = 1.76512.10^{-19}$ <second>, the two numerical relations for the chemical bonding field, namely (45) and (47b), are equated to give the typical lengths of the entanglement bond $X_{bond} \in (0, 3.19643.10^{-12})$ <*meters*> with a an observable character in the fine-structure phenomena ranges. On the other side, on a chemically femto-second scale, i.e. $t_{bonding} \sim 10^{-12} s$, one finds $X_{bond} \sim 10^{-8} m$ thus widely recovering the custom

length of the chemical bonding phenomena. Further studies may be envisaged from this point concerning the chemical reactivity, times of reactions, i.e. of tunneling the potential barrier between reactants, at whatever chemical scale.

Lastly but not at last, the relations (45) and (47) may be further used in determining the *mass of bondons* carried by the chemical field on a given distance:

$$m_{bondons} = \frac{\hbar t}{2} \frac{1}{X_{bond}^2}.$$ (48)

For instance, considering the above typical chemical bond length, $t_{bonding} \sim 10^{-12} s$ and $X_{bond} \sim 10^{-8} m$, one gets the bondon mass about $m_{bondons} \sim 5.27286.10^{-31}$ *kg*, of electronic mass order, of course, but not necessary the same since in the course of reaction, due to the inner undulatory nature of electron and of the wave-function based phenomena of bonding, the electronic specific mass may decrease. Note that the bondon mass decreases faster by broader the bond distance than the time providing a typical quantum effect without a macroscopic rationalization. In fact as increases the entangled distance to be covered by the chemical interaction not only the time is larger but also the quantum mass carried by the field decreases in order the phenomena be unitary, non-separated, and observable! Most remarkably, the higher limit of bondonic mass correctly stands the electronic mass $m_0 \sim 9.1094.10^{-31} kg$ as easily verified when the first Bohr radius and associated time are replaced in (48) formula.

With these the chemical bonding phenomena should be considered as completely described in the context of Bohmian quantum mechanics of electrons without spin. Spin inclusion requires a special separate study and will be communicated in the years to come.

4. CONCLUSION

Although not among the first ten great mysteries of the Universe, the chemical bond nature seems to subsist in many of them, especially in relation with the existence in a quantum world. As such, as far as the quantum mechanics opens the way for an entangled non-local picture of interaction between, in principle, all things in Universe the Chemistry–through its bonding level of manifestation–makes things discernable, observable and at the end measurable. In supporting this view the de Broglie-Bohm wavefunction was transformed, actually rotated in the complex space of phases with a quantity that was later shown to account for the chemical bonding field ▯ by means of consequences raised by

Schrödinger invariance condition under such U(1) transformation. There is remarkable that despite U(1) gauge transformation is well noted in the Yang-Mills transformation of fields that helps in explaining the symmetry broken by creation of elementary particle, this is the first study that addresses nonlocal gauge transformation on de Broglie-Bohm-Schrödinger wave fields, however leading with impressive result of identifying the chemical bonding field with observable quantity as electronic density and its gradients. Moreover, the existence of chemical ▯ fields implies that the entangled interaction in boning is carried by associate elementary particles called as bondons; they have lower mass than electrons for typical chemical bonding length having the electronic mass as the superior limit when the first Bohr radius is set as the bonding length. This way, the present work opens the possibility of unifying the chemical interactions through chemical bonding fields and associate bondons.

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