Chemical bonding as quantum tunneling: The Capra bondons

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ABSTRACT
The chemical bonding phenomenology is approached through the quantum tunneling rather than by the fashioned quantum wave function superposition/interference. It provides a complete covering character of the nano-space for topological chemical structures, which otherwise geometrically feature the space-gaps. The covering completion is actually recovered by the quasi-particle bondon as the information agent in filling the potential gaps of both asymmetrically and symmetrically extended or generally topologically reduced chemical structures. In such a context, we found that Prof. Diudea's Capra topological operation provides the bondonic quantum pentagulation, which resembles the nano-topological analogue of the Wigner-Seitz primitive in periodic lattices, while also establishing the direct connection with the reciprocal k-space of wave-vectors and with the allied Brillouin zones of electronic (bosonic) condensation.

1. Introduction

In nano-chemistry, nano does not refer *only* to the size of the studied objects, but also to the instruments with which these objects are investigated. For instance, *light* is nano by definition, especially in the regime of stimulated emissions (laser). Any molecular investigation with laser falls within the incidence of nano-chemistry, while *electrons*, for instance, with a radius of ca. 10^{-15} m are even sub-nano entities. Yet, the electrons-molecules interaction, or the electrons-atoms type constitute natural nano-systems, etc. Generally speaking, *investigation of matter with the help of matter* remains the major key of the nanoscopic approach, i.e., we can continue investigating the location of electrons with the help of electrons; establishing the distribution of electrons with the help of EM radiation, all types of wave-corpuscle interaction, including the wave-molecule interaction, along with ultrasonic experiments, even with microwaves (since they activate internal vibrational states for the studied molecules). Therefore, all of these are nano in their nature. On the other side, the *electronic-time* investigation, viz. the time of flights, goes with femto-spectroscopy, as in the 10^{-15} seconds optical recordings. The temporal (sub-)nano-scale is also specific to matter-matter interaction's timing (the corpuscle-corpuscle and the wave-corpuscle couplings), e.g., the lifetime of excitation-decaying, charge transfer, quantum tunneling, transmission of chemical information through electronic delocalization, chemical bond formation time, etc. All emphasize the nano-chemistry's investigative role in the matter with the help of matter research!

On the next level, nano-chemistry is going quantum. Why quantum? Because the main objects that the quantum custom wave-particle duality raise are celebrated as *quasi-particles*, e.g.,: the excitons (i.e., the set of excited particles in a state characterized by the same wave function, that is, more corpuscles are coherently linked by the same wave), plasmons, solitons (formed in assemblies of excited macro-molecules or intensive electromagnetic fields), and - with special interest in the inter-electronic couplings and in the chemical bonding-, the recently formulated chemical bosonic particles (the so called bondons). Anticipated since over a decade ago and then systematically applied to various chemical systems,[1,2] they conceptually answer to the primary question of chemistry, i.e., they offer the complete (wave-particle) explanation for the quantum nature of the chemical bond and bonding: *Why electrons, as fermions with the same negative electric charge, instead of repelling each other - as predicted by classical physical and chemical theory -, not only do not reject each other, but combine in lower/more stable energetic states, rather than the energetic states of the incoming electrons*? The answer raises naturally: the electrons, as fermions, actually couple in forming bosons in lower energy states, and therefore can co-exist on stable energy states in any number (viz. double, triple, and collective electronic bonds), while the boson particle that mediates the interaction between those fermionic electrons is represented by the quantum quasi-particle bondon B, see Figure 1.

Moreover, bondonic phenomenology allows for developing chemical fields in nano-carbon extended systems, including the mechanism of their photo-chemical sensitization through the quantum dots couplings, i.e., by generating

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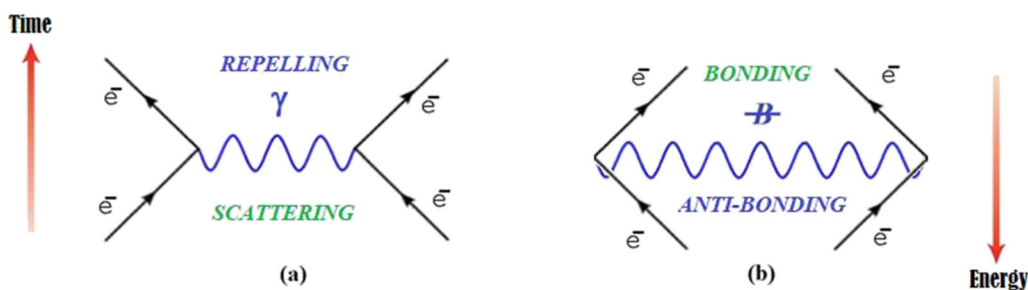
Figure 1. The bosonic interaction among fermions: a) inter-electronic repulsion in free state via bosonic-photons; b) inter-electronic bosonisation via bondons of chemical bonding for atoms-in-molecules; Time is indicated so that the Feynman diagrams can be accordingly followed in both photonic and bondonic bosonic quantum fields: driven by repelling and by binding phenomenology, respectively; On the other hand, the Energy arrow goes inversely: the pre-scattering and the anti-bonding states are at higher levels in photonic vs. bondonic interaction pictures, respectively.

the bonding of quantum-dots, the *bondotic* systems. As quantum quasi-particles, the bondots further mediate the interaction between nano-particles[3] at the quantum field level, which results in forces that equilibrate the states, either in meta-equilibrium or in excited configurations, respectively; they also transmit (they "communicate" in the sense of quantum information transmission)the interfering wave functions as wrapping of the bound system, while containing (within the wave-packet constructive interference) the entire history of the ensemble and its subsystems, at the atomic, molecular, and supra-molecular constitutive and fragmentary levels. It is such framework in which the current quantum topo-nano structure and information may be unfolded in an unprecedented way, with the aim of extending the nano- and carbon-like systems. Entanglement and space coverings as interrelated phenomena may be revisited as such from within the bondonic theory that advances by tunneling, rather than by interference of the constituents of the chemical bonding. This way, the present endeavor reports on the nano-space covering as it may be achieved by the aid of extended bondonic appliance.

Accordingly, this paper unfolds as follows. Section 2 presents the nano-space covering by quantum tunneling in the chemical bonding; Section 3 is an application to the bondonic case of the special Capra topo-nano transformation, which reveals for the first time a connection with the Brillouin/Wigner-Seitz primitive cell topological phenomenology; further discussions and perspectives are summarized in the Section 4 of the Conclusion.

2. Chemical bonding by topo-quantum tunneling

Quantum chemistry, despite its successful story, is still highly incomplete. Suffice it that one looks at how much attention the „old story renewed", as the Valence Bond Theory– VBT, (Shaik et al. 2021)[4] incepted by Pauling about a century ago, and which currently gathers huge interest from various aspects of atoms in molecule bonding, reactivity and properties, viz. Molecules 2021.[5] And all of these because the inner concept of (quantum) chemistry, the chemical bond and bonding, is incomplete. And it is incomplete because it misses the quantum closest path among particles and waves: the electrons of the atomic orbitals interact (via. constructive/destructive interference) to produce

molecular orbitals (as a special form of de Broglie wave packet). The associated respective and specific quantum particles remained unexplored. Naturally, *to the same extent that the electrons in their free state interact and repel via bosons as the photons*, the interacting-to-bonding electrons in a confined molecular space with the same energy should exchange their bonding information via **bonding bosons** (the so called **bondons**). This way, by tunneling, the *inter-electronic repelling Coulomb potential barrier (through specific bosons—the bondons) is passed through (back and forth)* and the molecular cohesion and structural stability is assured.[1] The mechanism is flexible enough to allow further reactivity and dynamics, up to formally covering the otherwise intricate Fock-space cluster theory, whichdeals with thecollective interaction of the interacting (excitations included) many-electronic systems.[6,7] While the "classical" chemical bonding theories have many virtues, they all feature some hidden concepts that prevent the revealing of the true nature of the chemical bonding (Figure 2). As such, while hybridization in VBT drawbacks from the fact that it advocates new (self)-produced orbitals without spectral correspondence, the anti-bonding orbitals in Molecular Orbital Theory—MOT—requires the conceptual odd picture whereby the inner orbitals in a molecule can be of a destructive interference nature, so they may affect the stability of the atoms-in molecules. Instead, the collectivization density functional concept of the Density Functional Theory (DFT) makes a truly firm step in allowing for a reinterpretation of the chemical bonding as a special case of the Bose-Einstein condensation.[2] It nevertheless further hinders the bosonic explicit tunneling mechanism of bonding through the DFT exchange-correlation formalism that "still preserves" (despite some "hole exchange" phenomenology also being employed) the fermionic nature of the whole ensemble of the many-electronic systems.

The Bondonic Theory, on the other hand, being still in development, has the virtue of boldly stepping toward a firm statement of the bosonic existence under the inter-electronic quantum fields in bonding, in accordance with the universal physical principle that fermions should interact via bosonic field(s), all within the full quantum theory prescription.

In order to be able to approach the structural chemical topology, one has to have a clear idea about the quantum definition of the 3 D Space. The 3 D space is the 2 D space
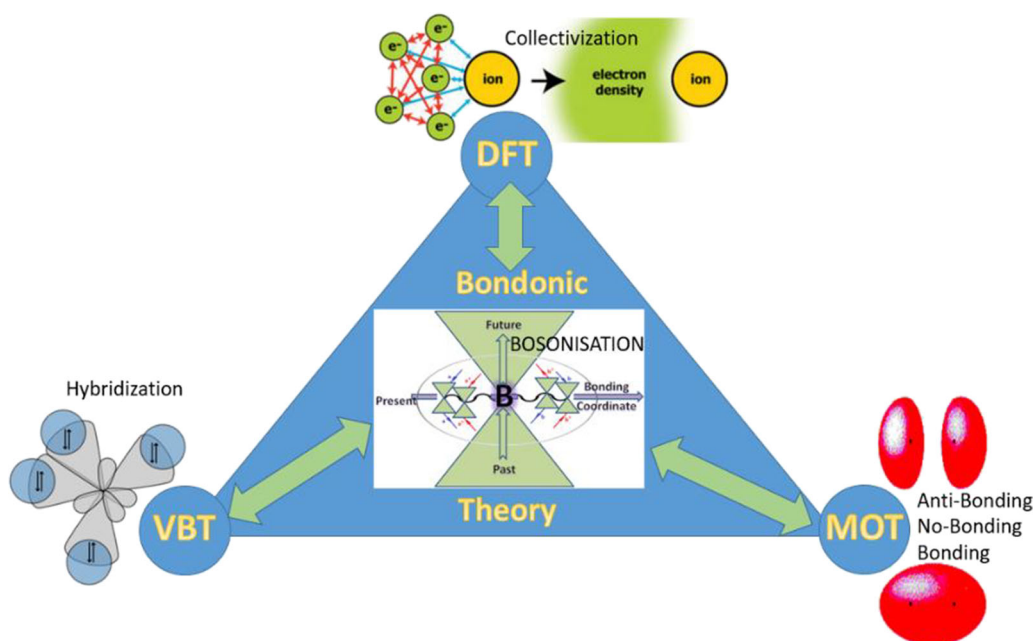
Figure 2. The theoretical tetrahedron with the actual four vertices representing the fundamental approaches of the chemical bond: VBT—the valence-bond theory—based on orbital hybridization; MOT—the molecular orbital theory—based on pairing bonding-antibonding orbitals, DFT—the density functional theory—based on electronic collectivization (via exchange and correlation), and the actual BONDONIC THEORY that advances the unification paradigm of bosonisation of the electrons in bonding; see the text for further details.

seen as an inverse "CORPICA" projection, which adds the 1 D space coordination for the wave (packet)-information! In other words, quantum-3D = 2 D-particle ("space spot/localization") + 1 D-waving (,,space covering by propagation/delocalization"). Note that the 1 D it is not necessarily the straight line or trajectories! In general, the 1 D is a universe in itself on a curved string! (See for instance, the limiting quantum string theory[8]). This way, the complete 4 D space = the 3 D—structural matter covering (with its substantial bodies and the corresponding waving information included) + the 1 D time "velocity" of such covering. In the Special Relativity theory, 1 D = Temporal information, as it is also an essential waving/propagation information, yet as a whole it accounts for the ,,propagation of propagation"! Also, in this case, it is worth mentioning that "time" is linear *only in the case of the non-inertial systems (in rest on themselves),* otherwise specific transformation (Einstein-Lorentz) beholds. Iteratively, through a generalized quantum-relativistic theory on any space, one may convey the dimensional decomposition *ND = (N-1)D of a corpuscular nature* ("the resting/substantial coverings of the space") + *1 D of an undulatory nature* ("the waving covering which complements the localization). At this point, wave collapses in the composite N × D system! Actually, the wave function collapses its wave packet into the particle through the so-called tunneling (either free or with potential filled space), Figure 3. Note that the Figure 3 does not depict orbitals of (symmetric/asymmetric) molecules –e.g., "two ethene molecules" -, yet the orbitals effectively tunnel a generally (asymmetric) potential barrier (so they produce an inversing in some of the orbitals' spins through tunneling) among various parts in a *generic* molecule (hence the HOMO/LUMO indication is added to point to the molecular realm)!

The quantum tunneling is indeed a special phenomenon because it includes self-creation and thus it assures either an orbital stability in a close system or a passage through the barriers or wells of potentials in open or composed/interacting systems. In the case of the chemical bond, the bosonisation theory of electrons in bonding was already advanced; fortunately, it can be consistently described by the quantum tunneling phenomenology. Consider in Figure 3 the two sides of the potential barrier as being the electrons in bonding; they communicate by quantum tunneling the potential barrier defined by the type of chemical adducts in bonding and widely correspond to the potential barrier naturally formed by the separate (repelling in the free state) particles with the same charging. However, such potential happens to be just the playground of the quantum tunneling of the same type of electronic information from one side of the barrier to the other. Thus, the formed potential barrier actually ,,condenses" the inter-electronic interaction, which corresponds to the forming and interacting of the specific boson—the bondon; in simple words, the ,,house of the bondon" is just the inside of the potential barrier which prevents the electrons tighten through their interaction; so the bonding that relies on electronic collectivization and pairing only takes place within the ,,peak of the repelling inter-electronic potential" by their mutual tunneling form one side to the other. Remarkably, such phenomenology is included in the original derivation of the bondonic mass.[1] Just consider that the tunneling wave takes the electronic amplitude of one side of the ,,repelling potential" entirely into the other side and further unfolds the wave information as the fine structure propagation inside the electronic containing structure; the bondonic mass will naturally result in a simple way. In analytical terms, we thus have:
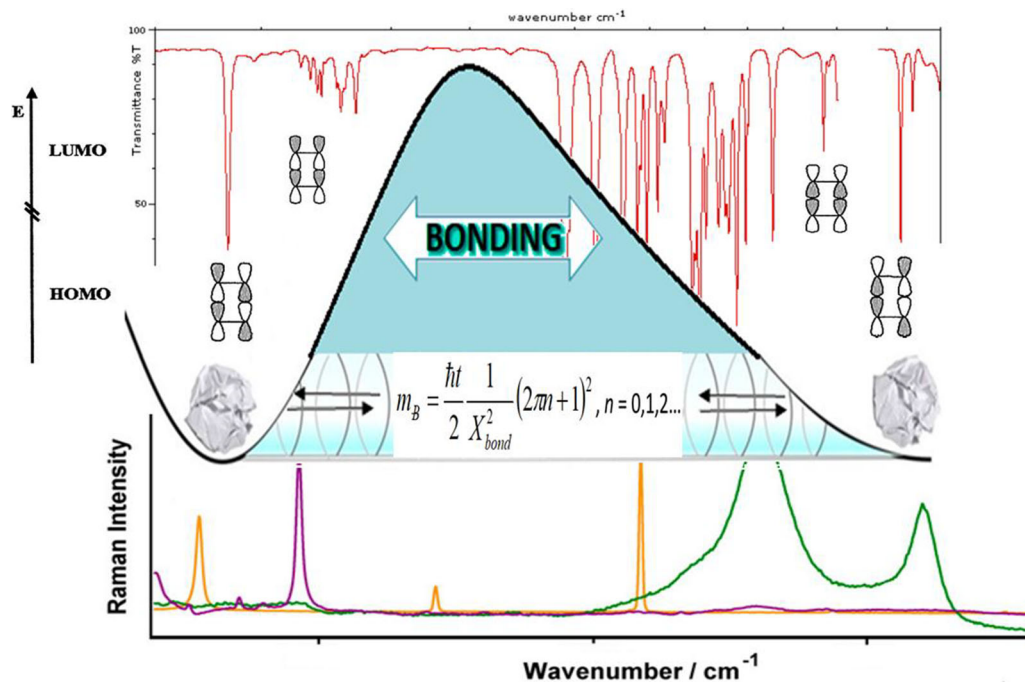
Figure 3. Quantum tunneling through potential barrier[s](viz. "the gaps in spectra") in a general many-particle bonding environments(here, incidentally, the barrier potential may be associated with the quantum spectral density of the states form, toward "quantum by quantum" measurements, observation and coverings): observing the bondons (B) as the quantum particles of the chemical bonding, which thus demonstrate their ontological existence, with the aid of FTIR (upper) and Raman (bottom) spectroscopy as applied to carbon order nano-systems (graphenic nano-junctions) and silicium materials (oxides, alloys), as complementary structural information; adapted upon[9]; see also.[10]

$$\begin{cases} \aleph B(t, X_{bond})\big|_{\substack{BEFORE \\ TUNNELING}} = \aleph_0 \aleph B(t, X_{bond})\big|_{\substack{AFTER \\ TUNNELING}} \\ = \aleph_0 \exp\left[-\frac{i}{\hbar}(pX_{bond} - Et)\right] \Rightarrow 1 = \exp\left[\pm\frac{i}{\hbar}(pX_{bond} - Et)\right] \end{cases} \tag{1}$$

that implies the quantification

$$pX_{bond} - Et = 2\pi n\hbar, \ n \in \mathbb{N} \tag{2}$$

Subsequently, one employs the Heisenberg time-energy saturated indeterminacy at the level of kinetic energy, abstracted from the total energy (to focus on the motion of the bondonic plane waves)

$$E = \frac{\hbar}{t}; \ p = mv = \sqrt{2mT} \to \sqrt{\frac{2m\hbar}{t}} \tag{3}$$

The bondon Equation (2) now becomes

$$X_{bond}\sqrt{\frac{2m\hbar}{t}} = (2\pi n + 1)\hbar \tag{4}$$

When solved for the bondonic mass, Eq. (4) yields the predicted expression:

$$m_B = \frac{\hbar t}{2} \frac{1}{X_{bond}^2}(2\pi n + 1)^2, \ n = 0, 1, 2..., \tag{5}$$

Equation (5) further rewrites through replacing the time with the associated Heisenberg energy, $t_{bonding} \to \hbar/E_{bond}$, thus delivering the "chemical bonding" working expression for the bondonic mass

$$m_B = \frac{\hbar^2}{2} \frac{(2\pi n + 1)^2}{E_{bond}X_{bond}^2}, \ n = 0, 1, 2..., \tag{6}$$

We have now the natural explanation of the fact that a *quantum mechanism is always quasi-quantum*: it always interchanges from a corpuscular and its undulating complement of the propagation to other or the same or augmented corpuscular *sub- or new- or quasi- systems*; the mechanism includes several waves which collapse through interference, tunneling, creation-annihilation, renormalization, asymptotically interaction ("long-range interaction"), multidimensional patterning (i.e., delocalization, entanglement), etc. Overall, the *quantum filling of space at the nanoscopic level is thus assured*!

However, the next important passage regards the merging of the geometrical space with the quantum tunneling paradigm; the key here is in the asymmetric geometries that produce specific types of "separating potentials"; such asymmetries are reflected in potential barriers or wells (the inner nature of a potential is to characterize a system by its spatial field of forces, either balanced—as in symmetric or specific potentials –, or not). Accordingly, *the quantum phenomenology of tunneling covers the nano-space inasmuch as the asymmetric potential's gaps are present in its periodic structure or in the contingency* (adjacency environments, baths, etc.)!

As a first illustration of the concepts, we give here the classical example of the geometrical imperfect coverage of space: the pentagons' tilling. While presenting gaps at the macro-level, when it becomes *nano-extended, the gaps act as intermission potentials that trigger the communication of the*
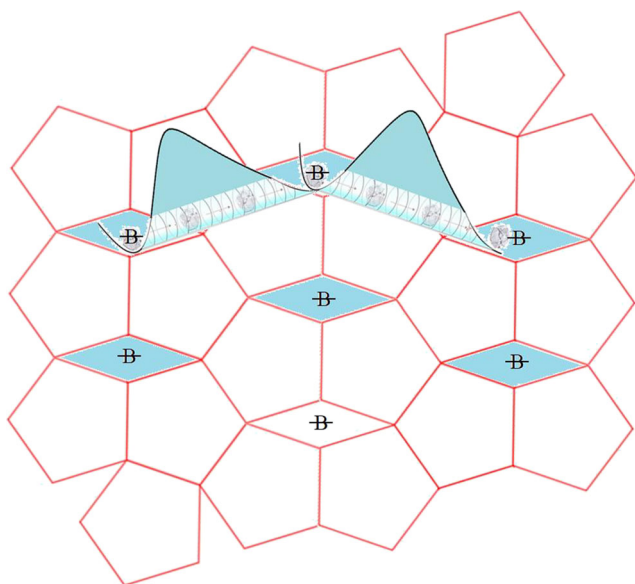
Figure 4. Bondonic quantum tunneling on a pentagonal "chemical bonding" tilling of nano-space—so assuring its entire filling even through its "potential" gaps; here the bondons are the bosons specific to pairing of two four-order nodes, each with two adjacent bonds in the nano-lattice.

Figure 5. The (6,3) covering in the toroidal and cylindrical embedding, respectively: (Left) (6,3)H/Z[12,50]; N = 600; (Right) Tu(6,3)A[12,12]; N = 144 in Schaefli notation[11].

quantum information present in adjacent pentagons. Figure 4 illustrates such a quantum mechanism for bondonic formation as a per tunneling phenomenon described in Figure 3 and above.

The consequences of such a perspective are immense: it actually opens the way according to which, at the nano level, the more mixed systems we have, the better they fill "their quantum lives": once they recognize and develop specific set up and development conditions that control the nano-topo-systems, the wave dynamics aim at the functionalization and the connection with other systems, the sub-assemblies, and the integrated systems for intelligent ("smart, sustainable") operation, with the appropriate design (and this is where *nano-technology* starts-up)!

Of course, one may further ask what happens with the nano-symmetric structures, even with the extended ones, such as the graphene? Well, here as well the asymmetry arises, at least from „two sources": one is due to the chemical isomerization that „covers differently", i.e., not globally symmetrical to the entire network with the same electronic conjugation patterning, i.e., the alternating of simple with double carbon-carbon bonds are not identically for any graphenic cells; it may have a periodicity, yet this is also the source of the „asymmetric wave" and hence the bondonic propagation through the graphenic lattice. But let's take the overall single bonded graphenic system, or a tori embedded (i.e., *drawing of a graph on a (closed) surface with no crossing lines*) nano-system as in Figure 5; and let's suppose the charge saturation or compensation applies either to the frontier of the system itself—as in the case of graphene, or the system is overall charged—in the case of the embedded tori. How do the asymmetries appear inside such a pristine network of linked hexa-carbon units? In this case, the second source of asymmetry arises: that is due to the topo-defects, e.g., the Stone-Wales rotations[11,12]: just because all the carbon bonds are identical in such a perfect lattice, their

equivalence, at the *quantum level of equivalence in inter-changeability of elementary particles, and thus also of bonds* can be inter-changed in equivalent rotational inner substructures. The asymmetric potentials have just risen, so the bondonic propagation begins as such as the (Stone-Wales) rotation topological defects move along the graphenic (initially pristine) lattice.[13,14]

For fullerenes, and other mixed types of nano-embed-ding—all with pentagon-hexagon carbon bonding combinations present -, it is clear that the third source of asymmetry is present, apart from the already recognized Stone-Wales rotation that can appear as a topological defect as well, just based on such adjacency that may be regarded as a penta-gon-hexagon bond, pairing the bondonic waves through the structures—when the new quasi-particle called bondot (bonding of quantum-dots/bondons, see also the introductory Section 1, and Ref. [3]) may be under purview and control (viz. quantum sensitization, thermo-effects without electric currents, or other nano-tech combinations thereof).

All in all, quantum tunneling is not a complementing, but a through covering mechanism at the nano-topo level of matter. Yet it has peculiar particularities; that implies that the type of symmetry/asymmetry of the pristine geometrical space of tiling is assumed. Such special case is to be described in the next section.

3. Quantum-CAPRA operation: Bondonic quantum pentagulation

We have just established that the topological dynamics are enhanced by the "wave-corpuscle" quantum dynamics, whereby the corpuscle = *basic/pristine structure*, and wave = *all topological forms are self-created, derived, propagated in/from the basic structure*. However, *the difference between nano-structural topology and nano-structural isomerization* appears to be in that the first is more correlated with the structure's dynamics based on the modification/displace-ment/rotation of the intrinsic chemical bonds (*edges* of/in the nanostructures); it also involves rearrangement, *displacement*, and the reordering of the atoms and molecules from the adjacent vertices in nanostructures (*vertices* of/in nanostructures)!

It is time now to illustrate a typical quantum connection of the nano-dynamics with the nano-structural topology. In particular, here we will choose the peculiar case of *Capra operation*, originally introduced by *Prof. Diudea* following a worthy suggestion of Prof. A. T. Balaban about the (Le[apfrog]) operation.[15,16] Capra (*the goat*) is the Romanian correspondent of the leapfrog English children
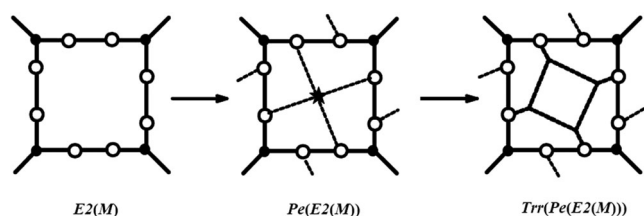
Figure 6. Capra as a sequence of elementary operations.

game; it will usually be symbolized as (Capra) Ca, and it follows the topological definition as such: *put two points of degree two on each edge of the map*, by an operation called E2[17]; then *put a vertex in the center of each face of M and make (1, 4) connections, starting with a two-valent vertex* –an operation called as *pentagulation* Pe, in analogy to the triangulation; the last operation refers to *a (reduced) truncation, i.e., by uniting the middle cut of each of the1-4 connections*; the successive operations resume as Ca(M) = Trr(Pe(E2(M))), with the effect in rotating the parent *s*-gonal faces by *p/2s*. The sequence above discussed is illustrated in the Figure 6.

Nevertheless, it is worth mentioning that the Ca operation is an enantiomeric pair of the object, since it is built up upon pentagulation over the alternating points of degree two, CaS(M): CaR(M) being a "racemic" pair, in the sinister-rectus chemical terms; as a convention, all non-specified Ca-transforms are considered as CaS(M). Yet, there is also another quantum consequence: since the Ca operation is basal on two-points of degree-two along a periodic primitive of the nanostructure, one is actually dealing with chemical bonding or with electronic pairing space over that which is imposed on the direct topological one. What follows seems to be a special version of the Wigner-Seitz primitive construction in the chemical bonding space; yet, it happens that the chemical bonding space of the quantum space of the electronic wave functions as a tunneling through the specific geometrical nano-structural barriers that drive the inter-electronic repelling; as we already presented in the Section 2, the chemical bonding is merely a quantum tunneling, rather than a quantum interference; the bosonisation of electrons as the resulting bondon of the Capra nanostructure is just the accumulation of quantum information of bonding within such pentagulation. It appears therefore that the pentagulation, although regarded till now just as an abstract nano-topological construct, it is in fact the pentagulation (a certain case of localization) for the chemical bonding quasi-particles—the quantum bondons on nanostructures.

This is an original result that enlightens the meaning of the Ca operation with the quantum condensation identification on nano-topo structures via pentagulation; this finding can make of the Ca operation a useful tool in assessing the chemical bonding space, that is, the bondonic maps in the topological nanospace. Fortunately, one direct consequence is also within reach. When considering the periodic lattice, for instance that of Figure 6, one may combine, also recursively, the supercells in the quantum nano-dynamics of the pentagulated bondons among their adjacent Ca locations, with the remarkable result of obtaining the Brillouin first

zone of equivalence, see Figure 7. From the one-to-one figures' superposition, it also appears that the bonding itself and the bondonic pentagulation thereof fulfills the atoms-in-molecule (AIM) Bader's zero flux density in the electronic space of bonding[20–22]

$$\nabla \rho_{AIM}(r)\,|_{R_{Bond}} = 0 \qquad (7)$$

Such condition may seem paradoxical at first sight, and was accordingly debated in the last decades,[23,24] i.e., the bonds are formed where their electronic flux of density vanishes, yet it actually corresponds to the pentagulation and it is consistent with the actual quantum tunneling process (which involves, as the quantum inter-level transitions, a sort of „quantum void passage", in fact the tunneling of the potential well/barrier); more straightly said, the quantum tunneling and the chemical bond themselves (the paring of electrons, which otherwise are naturally repelled) may be regarded as a special case of quantum entanglement. This is yet to be detailed in another forthcoming communication.

However, what we phenomenologically obtained is of prime importance in quantum chemistry in general and in the chemical bonding theory in particular; we actually opened a way of mapping the chemical bonding information inside a nanostructure by performing its nano-topological analysis through the Capra transformation and pentagulation. Even more, the actual results also emphasize the topological correspondence between the direct chemical nano-space and the quantum space of the chemical bonding, without the celebrated k-space analysis and the allied X-ray or reciprocal space transformation (viz. the dual space). We arguably reached the conclusion that chemical bonding alone, when treated as a quantum quasi-particle bondon, in its turn resulted via quantum tunneling, actually performs the direct-to-quantum morphism that is able to provide the „localization of the delocalization", i.e., the electronic bosonisation in bondons of chemical bond and/or the quantum condensation of the collective wave-function of a given nano-structure in its topological quantum-dots via pentagulation; and the Ca operation is the corresponding link.

Eventually, the Q-Capra pentagulation may trigger also the allied quantum electrodynamic set-up, i.e., the designing of the specific nonlinear optical lattice wherein, by trapping a given nano-chemical structure, one can map the „condensed/dotting/bondonic" chemical bonding information and further control or entangle it by/within the next generation of quantum molecular computation, coding, or other unforeseen use as of right now.

4. Conclusion

The quantum nano-chemistry just opened its frontiers at least by two folded reloaded main themes of chemistry: bonding and reactivity, which both lead the new age of artificial and exotic synthesis, from carbon-extended systems to molecular machines, quantum information and computing. The chemical bonding itself remains one of the major paradoxes of physics; it is not completely unveiled by the quantum mechanics. It requires an explanation as to how
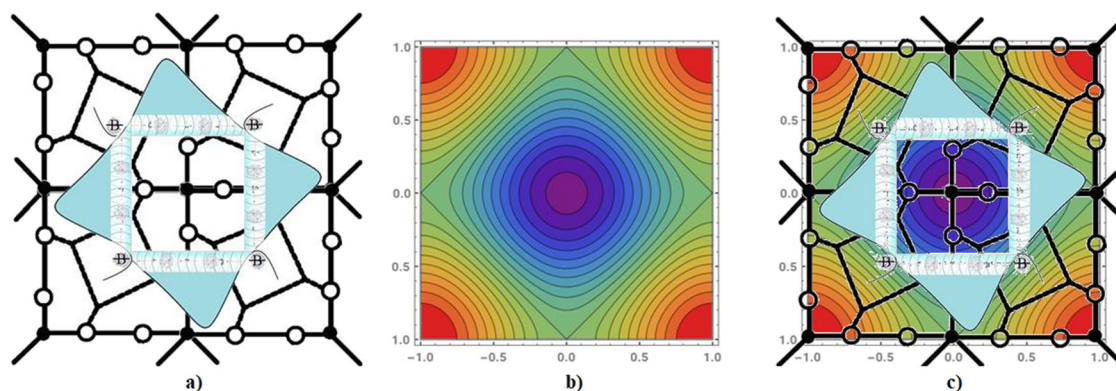
Figure 7. a) Quantum Capra-pentagulation by bondonic tunneling the chemical bonding bosonic information vis-à-vis b) the s-band dispersion relation for2D lattice under tight binding approximation in the first extended Brillouin zone/Wigner-Seitz primitive,[18,19] and c) their superposition for a periodic lattice (black balls); see text for further details.

identically charged particles not only do not repel, but they also pair in stable levels, even bellow the adducts' incoming electrons in chemical systems! Therefore, the present endeavor belongs to the last decade's efforts of rethinking the quantum nature of the chemical bond. According to the present contribution, it appears to be merely related to the quantum tunneling, rather than the quantum interference, or with both (yet in this order, in an entangling manner).While quantum superposition explains wave-function interference and predicts the resulting bonding-antibonding, i.e., the entire molecular spectra, by solving the eigen-value problems in more and more sophisticated (perturbative and coupled clustering) ways,[6] the non-repelling explanation remains unsolved, unless the mutual tunneling and the bosonisation of the interacting electrons is being considered.[25,26] Such tunneling phenomenology consistently covers the quantum space of the atoms-in molecules right there: through the local barriers or through the repelling potentials. The chemical bonding space is therefore associated both with the covering of the nano-space by wave-packet tunneling, and with the providing of the quantum access to the inner space of the k-points (the wave-vector frontiers), and the zero density fluxes' contours that define such bonding. The present communication exposes in a consistent, heuristic manner such complex, yet insightful paradigm as the following: the quantum space of the chemical bonding complements and covers the nano-space of the chemical topology, either by filling the asymmetrical potential gaps or by accompanying the asymmetrical dynamics raised on the symmetric lattice just because of the topological defects created by the interchanging of otherwise equivalent bonds in pristine lattices. The specific Capra operation was identified as the simple, direct, and possibly universal pentagulation, i.e., localization, of the bondonic information on a given chemical structure (represented by its graph). That appears to be consistent with the tunneling phenomenology, while it recovers the zero flux Bader's density condition of bonding and fitting with the Brillouin first zone of reciprocal space for periodical lattices. Therefore, there is much hope that such epistemological venture continues toward a closing of the physical-chemical theory of bonding and a binding in a consistent quantum phenomenology. This is also a great opportunity for linking the meaning of the chemical graph theory,[27] and the chemical mathematical topology treatment with the quantum information and its proper design.

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