

A unitary model for atomic structure

S. K. Balasubramanian,

B-8, Apsara apartments, 259, Bund Garden Road, Pune 411001, India.

Summary: In the unitary model the atomic nucleus plays a decisive role in atomic structure and atomic interactions including chemical bonding.

Abstract: On the assumption that nuclear structure determines and dictates atomic structure and molecular geometry, structures for Carbon, Silicon, Boron and Chlorine atoms are proposed that explain their covalent bonding patterns. Arguments are presented against the current interpretation of “atomic number”.

The text of the article

These deductions have serious bearing on the quantum mechanical bicameral model ¹ for atomic structure based on the assumption that there are two independent parts in an atom, namely, the nucleus and the electronic parts. Wave particle duality is essential to rationalize the concept of orbitals for electrons. The aufbau model is based on the assumption that the nucleus is no more than a point charge that holds the electrons together in the atom.

In this paper we present evidence from the chemistry of Carbon, Silicon and Boron for an alternative unitary model for atomic structure based on the following assumptions:

1. Every nucleus is composed of particles of uniform size known as nucleons. Following Linus Pauling ² we may say that the nucleons may have masses of one, two or three. The heavier particles were called dineutrons or trineutrons.
2. Nuclear geometry dictates and determines molecular or atomic geometry. This assumption makes the model “unitary”. The implication is that corners

and projections may be the covalent bonding sites. Nuclear models are treated as atomic models in what follows.

The following corollary of assumption number 2 may be deduced:

Charges (or electrons) may “rise from and subside into” the nucleus according to context.

This corollary is likely to meet with opposition from specialists. So we are devoting some attention to it.

We would like to clarify that the ‘rise and subsidence’ of electrons is different from beta decay. It is a low energy phenomenon and does not involve any nuclear rearrangement like beta decay. We are also not sure if electrons are involved in the process. Most likely, “electrical charges” are involved. We are using the term “electron” interchangeably with the “charge” associated with it.

The implication is that there is no permanent presence of a fixed number of electrons in an atom, like 92 in the Uranium atom. This conclusion is justified because uranium hexafluoride should have 86 non-bonded extra-nuclear electrons. It could not be a gas at any temperature much less at as low a temperature as 55°C. In the event, atomic number gives the position of the element in the periodic table without any implication as to the number of electrons in the ground state of the atom.

Variable electron count around a central atom is indicated in several other gaseous inorganic binary fluorides³. In a gas the intermolecular interactions are minimal. This should be so even in multi-electron systems like uranium hexafluoride with 86 non-bonded electrons in the inner shells and 6 pairs of bonded electrons. UF₆ is the heaviest binary molecule and its property of being a gas above 55° C shows that it may not have all the 86 non-bonded electrons on the central atom as required by the aufbau model. The presence of non-bonded electrons on the central atom is not compatible with its gaseous nature.

BF_3 , CF_4 , SiF_4 and GeF_4 are all gases with sub-zero boiling points though they have two or more non-bonded electrons. The fluorides of fifth group elements, Phosphorous and Arsenic, show more bizarre behavior. Besides being gases the trifluorides are acceptor ligands and the pentafluorides are Lewis acids (electron acceptors). The two elements are normally electron donors. The donor property is best brought out in Gallium Arsenide where the Arsenic atom donates a pair of electrons to the acceptor Gallium. If such an atom with a surplus of electrons becomes an electron acceptor we have to look for a far-reaching change in the electron count consequent on formation of fluorides.

The hexafluorides of Sulfur, Selenium and Tellurium confirm the trend. These are gases besides being dielectrics. The last property shows that electron effects are totally and measurably absent in these molecules though all three elements have 10 non-bonded electrons in the outer shells.

The property is not restricted to fluorides. Nickel tetracarbonyl is a gas above 30°C though Nickel has six non-bonded electrons in the carbonyl. These examples show that the electron count on an atom may be variable and support our contention that Moseley result ⁵ should be interpreted with caution and circumspection.

The Bohr model predicted proportionality between Z^2 and the characteristic frequency of the x-ray emission, Z being the number of extra-nuclear electrons. The plot of Z^2 against frequency should be a straight line. It was not found to be so. $(Z-1)^2$ gave straight-line plot. The explanation before 1980 ^{4a} was that an electron dropped into the nucleus to give an effective atomic number of $(Z-1)$. After 1980 ^{4b} Z is plotted against the square root of frequency. A straight line is got and is presented as proof of the validity of the concept of atomic number.

This is obfuscation of an excellent experimental result. The change from Z^2 to Z

is in effect a compression of the ordinate. Any set of results may be made to give a straight-line graph by suitable compression of the ordinates.

So one could say that the Moseley results show a correlation of the characteristic frequency of x-rays with the arrangement of the elements in the order of increasing mass numbers. The quantitative correlation of atomic number and nuclear charge should be considered open to question. Besides the generation of x-rays is a high-energy process that is not clearly understood. It should not be made the basis for such a far-reaching conclusion.

Chemical bonding or other interactions take place at the sites where 'rise and subsidence' of electrons take place. We are not commenting on the nature of the chemical bonding except to say that electrons need not be the binding particle in a chemical bond.

The bonding sites may be divided into the primary bonding sites, called b-surfaces and painted red. Secondary bonding sites are called the quiescent surfaces or the q-surfaces (yellow). Bonds involving the b-surfaces, b-b bonds, are the most stable followed by b-q, and q-q bonds.

Dineutrons may be implicated in electropositive elements like the alkali and alkaline earth metals. The positive charge is localized in the cation. Electronegativity is for the present left undefined. The negative charge may be evenly distributed around the central atom like F in a fluoride.

Inert gases might not have any extra-nuclear electrons or centers where the charge may rise and subside. Elements heavier than Helium may be composites of Helium nuclei and of other so far unknown inert elements like an octahedron of mass number 6 or an icosahedron of mass number 12. The last two might be chemically inert because each of the nucleons is bound to four or more nucleons.

Thus ^{20}Ne could be a composite of 5 atoms of ^4He . ^{22}Ne could be 4 atoms of ^4He + octahedron.

Periodicity is due to structural similarity or due to a common scaffold. Carbon and Silicon have tetrahedral bonding sites though their scaffolds are different. Fluorine and Chlorine and even manganese are built on the same scaffold.

Carbon

Carbon with 12 nucleons (^{12}C) is assigned structure (1). This is built from an octahedron, colored blue. All the positions on the octahedron are equivalent. Addition of six more nucleons at triangular sites gives ^{12}C with four nucleons at tetrahedral positions and two at tetrahedral sides.



(1)

(2)

Examination of (1) shows that there are three possible ways in which carbon can form four single bonds. The most stable of these is the tetrahedral pattern (red surfaces). The second possibility is a square pattern (2 red and 2 yellow) found in carbon monoxide and in an iron bare-carbon complex ⁵. The third possibility is one with three b-surfaces and the q-surface at the center of the tetrahedral face. This unique pattern is found in a compound called propellane ⁶ and shaped like a propeller. Quantum model is not compatible with the existence of this compound.

The tetrahedral pattern explains molecular chirality. Molecular chirality is not compatible with the quantum model. This is the most important objection ⁷ to the quantum model and the wave nature of electron.

Two possibilities exist for C-C double bonds (2). One of these is the common double bond, called the van't Hoff double bond, with shared edges. Another higher energy double bond with tetrahedral geometry is also possible. It is found in cyclopropene and accounts for its perplexing bonding propensities ⁸. The platinum complex of ethylene known as Zeisse's salt ⁹ is another example of a tetrahedral double bond.

There are two possible triple bonds (3) on the unitary model. The face-sharing triple bond with linear arrangement of substituents is shown on the right. The other triple bond is the b-b, b-b, q-q bond on the left. This is found in benzyne intermediate and is responsible for aromatic stabilization. ¹⁰



(3)

The new triple bond could show *cis*, *trans* isomerism. The *trans* isomer is known as an intermediate. ¹¹

Silicon

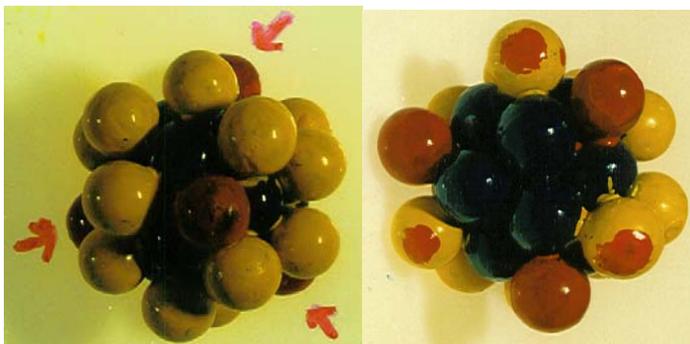
Silicon shows tetrahedral bonding similar to carbon. In addition it must have asymmetry at the atomic level since quartz shows solid-state chirality ¹².

The current 'explanation' of solid-state chirality depends on analysis of symmetry elements of the crystal structure. We dismiss such analysis as merely a description of the phenomenon and not an explanation.

To provide for chiral structures we postulate an icosahedron as the underlying structure for ²⁸Si. Sixteen nucleons are added to an icosahedron to get (4a and 4b) for ²⁸Si. The icosahedron part is colored dark blue. The apex and the tetrahedral parts are colored red in 4a. There is another set of tetrahedral surfaces in relation to the apex. These are colored yellow with red patch in 4b. The two tetrahedral structures are chiral to each other. They account for the

chirality of quartz. Tetrasubstituted silicon derivatives like SiR_4 could all exhibit solid-state chirality. They would not show chirality in solution since the chiral structures would rapidly equilibrate in solution by bond shifting.

Chiral equilibration without structural change is not possible in molecular chirality. This unique phenomenon is illustrated in the solid-state chirality of sodium chlorate. The chiral solid undergoes equilibration in solution and loses its chirality.



4a

4b

One could derive three more structures by shifting the apex nucleon and the three nucleons around the apex in (4a) to vacant places in (4b). All structures would show chiral behavior similar to (4).

Structural isomerism in an isotope is a new postulate. We suggest the name Siomerism for the phenomenon since Silicon is the first element identified to exhibit it.

Decamethyl Silicocene is known¹³. The pentad surfaces shown by arrows in (4a) account for this. In solid state the compound exists in linear and angular forms in the ratio of 1:2. The unitary model is in agreement with this ratio.

Boron

Boron, ^{11}B , is given structure (5a) which is a truncated Carbon without the tetrahedral apex. Boron shows four penta-covalent bonding patterns that are responsible for the formation of crystalline Boron containing interlinked icosahedral Boron atoms.

Diborane, B_2H_6 , is shown in (5b). There is $\text{B}=\text{B}$ (q-q) double bond. Hydrogen atoms are located on the red surfaces. The unitary model is the only model that accounts for this unique bonding pattern.



5a

5b

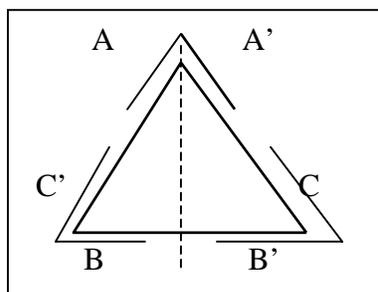
Chlorine

Chlorine (6b) is built on the fluorine scaffold (6a). The straws indicate the site at which oxygen is attached by quadruple bond in chlorate anion of sodium chlorate.



6a

6b



6c

Fig 6c shows the schematic arrangement of bonds marked by straws in 6b. A, A'; B, B' and C, C' are chiral pairs of bonding areas. When the bonds switch from A to C', B to B' and C to A' without breaking away using the common site (white straw in 6b) as the fulcrum equilibration of chiral forms takes place¹⁴.

The unitary concept had been extended to elements of the first two periods of the Periodic table such as ${}^6\text{Li}$, ${}^7\text{Li}$, ${}^9\text{Be}$, ${}^{14}\text{N}$, ${}^{16}\text{O}$, ${}^{19}\text{F}$, ${}^{23}\text{Na}$, ${}^{24}\text{Mg}$, ${}^{27}\text{Al}$, ${}^{31}\text{P}$, ${}^{32}\text{S}$, and ${}^{35}\text{Cl}$. In addition elements like Cr, Mn and Fe have yielded new insights

Further experimental work:

The following possibilities for experimental work are evident. We had initiated experimental work on chirality of nitrogen based on reported solid-state chirality of ethyl ammonium iodide ¹⁵. We had observed small rotation of both signs in solution. The work needs to be confirmed and extended.

Oxygen may exist as 4 isomers. Out of many combinations possible for molecular oxygen only one form would show paramagnetism. This property could be used to separate the isomer.

By careful choice of conditions it should be possible to observe rotation in solution of chiral solid sodium chlorate.

References:

1. E. U. Condon, in Handbook of physics, E .U. Condon and H. Odishaw, McGraw-Hill Co., (1967), sec 7.
2. L.Pauling, Science,1965,150, 297.
3. D.M.P. Mingos, Essential trends in Inorganic Chemistry, OUP, 1998
4. a. Arthur Beiser, Concepts of Modern Physics, Tata-McGrawHill, 2004;
b. W. E Burcham, Elements of Nuclear Physics; Longman, 1979.
5. N. N. Greenwood and A. Earnshaw, Chemistry of the Elements, , Pergamon Press, 1988.
6. K. B. Wiberg, Accs. Chem. Res. 1984, **17** 379. K. B. Wiberg , J. Amer. Chem. Soc., 1983, **105**, 1227; P. Chakrabarti, P. Seiler, J. D. Dunitz, A.

- Schuler, and G. Szeimes, J. Amer. Chem. Soc., 1981, **103**, 7378.
7. R. G. Woolley, J. Amer. Chem. Soc., 1978, **100**, 1073; S. J. Weininger, J. Chem. Ed., 1984, **61**, 939.
8. F. H. Allen, Tetrahedron, 1982, **38**, 94; W. E. Billups, Accs. Chem. Res., 1978, **11**, 245; W. Ando, Y. Hanyo, T. Takata, and K. Ueno, J. Amer. Chem. Soc. 1984, **106**, 2216. G. Szeimes, J. Harnish, and O. Baumgartel, J. Amer. Chem. Soc., 1977, **99**, 5183; U. Seebach and G. Szeimes, J. Amer. Chem. Soc., 1978, **100**, 3966.
9. R. Hartley, Angew. Chem. Int. Ed., 1972, **11**, 596. See R. Mason, Chem. Soc. Revs. 1972, **1**, 431 for a detailed discussion.
10. G. R. Davis, W. Hewertson, R. H. B. Mais, P. G. Owston and C. G. Patel, J. Chem. Soc. A **1970**, 1873.; J. O. Glanville, J. M. Stewart, and S. O. Grun, J. Organometallic Chem., 1967, **7**, 9.; W. G. Sly, J. Amer. Chem. Soc., 1959, **81**, 18.
11. R. Bergman, Acc. Chem. Res., 1973, **6**, 26.
12. A. F. Wells, Structural Inorganic Chemistry, 5th ed., (1984) p.1006.
13. P. Jutzi, D. Kanni, and C. Kringer, Angew. Chem. Int. Ed., 1986, **25**, 164.
14. D. K. Kondipudi, R. J. Kaufman and Nolini Singh, Science, 1990, **250**, 975; R. M. Pagni and R. N. Compton. Crystal Growth and Design 2002, **2**, 249.
15. F. C. Phillips, Introduction to crystallography p 123, fig.191; see also A. M. Glazer et al., Acta Crystallographica (1992). **B48**, 16-21; ibid., (1994), **B50**, 425-431.

Skb.

The following is not for publication. This is an informal discussion of the failures of Quantum Mechanics in Chemistry. The need for this is given under the subtitle "Justification".

S. K. Balasubramanian. Ph. D.,
B-8, Apsara Apartments,
259, Bund Garden Road,
Pune 411 001. India
Phone: + 91(20) 26120627.
E mail <smanian @sancharnet.in

Unitary Model for atomic structure-

CRITIQUE OF QUANTUM MECHANICS IN CHEMISTRY

(Justification for this critique: The major failures of Quantum Mechanics are in chemistry. These had been overlooked because of the notion, attributed to P.A.M.Dirac, that QM solves ALL the problems of Chemistry and major parts of those in Physics. The difficulties in application to Chemistry are not simply a matter of complicated mathematics involved in the process. There are severe problems of elementary logic. The problem may be indicative of a deeper malaise. It may be the basic premise of QM itself that is questionable. We leave it open and limit ourselves to the deficiencies in the application of QM to Chemistry.

The citations below are mostly to books. The concepts under criticism are part of the School curriculum the world over. They are not abstractions found in fringe literature; hence the importance of the Critique.)

*Part I S. K. Balasubramanian, Science submission no. 110075

Part II S. K. Balasubramanian, Science submission no. 116288

ABSTRACT: (Word count 63) The difficulties are dealt with under the following heads:

1. Chirality of molecules and molecular systems: Molecular chirality is incompatible with QM.
2. Aufbau model and its application to chemical systems

3. Molecular systems: ad hoc approaches
4. Electric Current and magnetism
5. Inert Gases, superconductivity and Meissner effect
6. Cold fusion
7. Proton sites and nuclear structure
8. Central dogma

Critique of Quantum Mechanics in Chemistry ¹

1. Chirality of molecules and molecular systems.

Chirality is the phenomenon in which molecules having an asymmetric center are known to exist in non-superimposable mirror image forms. Thus glyceraldehyde is known to exist as left-handed and right-handed molecules. These molecules are separable and are capable of independent existence. They are identical in all respects except the direction in which they rotate the plane of polarization of plane polarized light. The property is known as optical activity. Chiral systems are fundamental in biology. In entirety life molecules are based on a single chiral sense.

A 1978 paper published in the Journal of the American Chemical Society said that QM does not permit chirality ^{2a}. In a conference held five years later it was concluded that QM applies only to a single molecule and not to a collection of molecules ^{2b}. A single Chiral molecule, if isolated, would lose its chirality. This is strange, to say the least. For all practical purposes we have to take it that chirality is not compatible with QM. The most fundamental phenomenon of Chemistry is not accountable on the QM.

2. Aufbau model and its application to chemical systems.

The aufbau model³ is central to Quantum Chemistry. It postulates that a certain number of electrons determined by the atomic number occupy extra-nuclear space governed by the exclusion principle. The support for this comes from the interpretation of atomic spectra as transitions from one set of atomic energy levels to another. Problems arise in chemistry in the detailed examination of the energy levels known as orbitals and their shapes.

2.1. Carbon and tetrahedral carbon atom

Carbon is known to be quadrivalent and has a tetrahedral structure. The aufbau model would lead to an atom with a configuration $1s^2, 2s^2, 2p^2$. Ideally this atom is divalent against the observed tetravalency of carbon. To account for the higher observed valence, it is assumed that the orbitals undergo either hybridization or form molecular orbitals at the time of formation of molecules⁴. The change looks innocuous but is highly irrational. It means equating inequalities. The 2s and 2p orbitals differ in energy and orientation. They cannot be equated whatever the acceptability of the Mathematical procedure. It violates the essence of logic. Bond formation is a primary phenomenon. There cannot be compromise or equivocation at this fundamental level.

In another case we would be postulating a valence of five for one compound of carbon. This would entail the use of one of the 'inner' electrons for bonding which is not allowed in the aufbau model. Such pentavalency is allowed on our unitary model. The division of the extra-nuclear electrons into groups of 'inner' and 'valence' electrons is not rational and exceptions are found throughout chemistry.

The aufbau model with the distribution of electrons around the nucleus is clearly in error. Since the exclusion principle is inviolable we have to suspect that either the assumption of the presence of electrons in extra-nuclear space or the number of electrons around the nucleus may be the source of error.

2.2 Beryllium-Argon

Beryllium poses a different problem ³. It has the electronic configuration $1s^2, 2s^2$. With closed shells it should be inert. But the element forms simple and complex compounds, because, as is commonly explained, it has a vacant 2p shell. The reverse of this problem is found in Argon. It has a configuration $1s^2, 2s^2, 2p^6, 3s^2, 3p^6$. The 3d shell is vacant. By analogy with Beryllium, Argon should be reactive. It is not.

2.3. Argon-Potassium

Argon has a vacant 3d orbital ³. We know by analogy with Lithium and Sodium that the next element Potassium in the group should have one s electron. So here the convenient assumption is introduced that the 4s shell is of lower energy than the vacant 3d shell. The assumption leads to a circular argument, namely, an assumption treated as an explanation. The situation is worse in the successive period breaks after the higher inert gases.

2.4 Atomic number and periodicity.

The interpretation of atomic number or the position of an element in the periodic table as the number of extra-nuclear electrons depends upon Moseley's excellent work ⁵ on the characteristic frequency of X-ray emissions by elements. Bohr model predicted proportionality between Z^2 and the frequency of the emission, Z being the number of extra-nuclear electrons. The plot of Z against frequency should be a straight line. It was not found to be so. $(Z-1)^2$ gave straight-line plot. The explanation before 1980 was that an electron dropped into the nucleus to give an effective atomic number of Z-1. After 1980 Z is plotted against the square root of frequency ⁶. A straight line is got and is presented as proof of the validity of the concept of atomic number.

This is obfuscation of an excellent experimental result. The change from Z^2 to Z is in effect a compression of the ordinate. Any set of results may be made to give a straight-line graph by suitable compression of the ordinates. So I would say that the Moseley results show a correlation of the frequency of x-rays with the arrangement of the elements in the order of increasing mass numbers. The Correlation of atomic number and nuclear charge should be considered open to

question. Besides the generation of x-rays is a high-energy process that is not clearly understood. It should not be made the basis for such a far-reaching conclusion.

2.41- Inorganic fluorides and number of electrons in an atom.

The inorganic fluorides ³ present an interesting picture. Many fluorides are gases. In a gas the intermolecular interactions are minimal. This should be so even in multi-electron systems like Uranium hexafluoride with 86 non-bonded electrons in the inner shells and 6 bonded electrons. Even the formation of the covalent fluoride should be a matter of surprise as the outer shell electron orbitals ($Rn, 6s^2, 5d^1, 4f^3$) have to hybridize themselves to form 6 equivalent orbitals. UF_6 is the heaviest binary molecule and its property of being a gas above $55^\circ C$ shows that it may not have all the required 86 non-bonded electrons on the central atom. The presence of non-bonded electrons on the central atom is not compatible with its gaseous nature.

BF_3 , CF_4 , SiF_4 and GeF_4 are all gases though they have two or more non-bonded electrons. The fluorides of 5th group elements, Phosphorous and Arsenic, show more bizarre behavior. Besides being gases the trifluorides are acceptor ligands and the pentafluorides are Lewis acids. The two elements are normally electron donors. This property is best brought out in Gallium Arsenide where the Arsenic atom donates a pair of electrons to the acceptor Gallium. If such an atom with a surplus of electrons turns to be an electron acceptor we have to look for a far-reaching change in the electron count consequent on formation of fluorides.

The hexafluorides of Sulfur, Selenium and tellurium confirm the trend. These are gases besides being dielectrics. The last property shows that electron effects are totally and measurably absent in these molecules. Selenium and Tellurium have 10 non-bonded electrons in the outer shells.

The property is not restricted to fluorides. Nickel tetracarbonyl is a gas above $30^\circ C$ though Nickel has six non-bonded electrons in the carbonyl. These examples show that the electron count on an atom may be variable and support

our contention that Moseley result should be interpreted with caution and circumspection.

In other words electrons or charges may 'come and go' or, as we prefer to say, 'rise and subside' in an atom. We use the vague expression electrons or charges purposely because we do not know for certain if electrons are involved in chemical bonding. The phenomenon of 'rise and subsidence' of electrons or charges is different from beta decay that involves a rearrangement in the nucleus. Soddy's law of radioactive decay does not apply here. We are dealing with an atomic and not a nuclear phenomenon. In all probability the rise and subsidence of charges is mediated by the weak force. At present we cannot say more.

2.5 Orbital shapes:

There are only three dimensions in Space. These are exhausted with the p orbitals for any atom. With higher orbitals the shapes become bizarre ⁴. They are mathematical constructs and there is no way to realize their reality in physical shapes. The difficulty arises from having to account for the atomic number and exclusion principle together. The two together form a rigid cage from which there is no escape for the theory. The doubtful factor in these cases is the number of electrons on an atom in the context of molecule formation.

The problem may be due to the realities of Chemistry where everything fits into a structure. An unstructured or an abstract mathematical formula has no relevance in Chemistry.

3.Molecular systems: ad hoc approaches

3.1 Zeisse salt

Zeisse's Salt is a platinum complex with ethylene ⁷. It represents the worst case of ad hoc assumption in the application of QM to Chemistry. It is our criticism that every time a new bonding phenomenon comes into view a fresh ad hoc assumption is necessary to account for it. Such assumptions are without any basis in theory or experiment. They are anathema to our concept of a theory and are what may be called Procrustean methods after the Greek mythological

character Procrustes who would fit his guests to a cot of fixed size and chop off protruding portions or pull parts that fall short. In more popular language one would call it a shifting of goal posts. Such usage is permissible only in Alice in Wonderland. Theoretical inconveniences should be confronted and not plastered over or ignored.

For Zeisse's salt a new bonding mode known as the " σ (sigma) donation - π (pi) back donation bond" is introduced. The carbon atoms of ethylene do not have any more electrons for bonding without opening up the double bond. With the double bond intact in Zeisse's salt, the carbon atoms have to participate in a new bond of the above type. This bond violates all sense of logic. It postulates free energy release where none should be possible. When one goes from A to B and returns to A, it is common sense that there should be no energy change irrespective of the path/s followed. This σ -donation- π -back-donation bond demands that such transit, A-B-A, should lead to an energy gain. It justified the conclusion with mathematics. It should make perpetual motion close to realization.

3.2 Propellane

Propellane (C_3H_6) is a small molecule of great importance⁸. It has the shape of a propellor with an axis. The axis must be a chemical bond since the compound has proven existence and stability below 100°C. But theory does not allow the bond to exist. The problem arises because in propellane the axis bond cannot be a tetrahedral bond. In the latter the bonds radiate from the central atom to the corners of a tetrahedron. In propellane axis the bond is like the handle of a triangular umbrella with all the bonds facing the same direction. The propellane axis bond is called an "inverted bond".

In this case there is no room even for ad hoc assumption. The theory breaks down totally.

The breakdown of theory in propellane has implication for another fully documented property of the carbon atom, bimolecular nucleophilic substitution. This property is ubiquitous in and exclusive to carbon chemistry and had been exhaustively studied for over 100 years. If there cannot be electron density in the direction of the inverted bond, substitution reaction should not occur. Indeed it is known not to occur with other elements.

3.3 Boron

Boron chemistry is another case of total breakdown of theory. Boron should have 5 electrons or the configuration $1s^2, 2s^2, 2p^1$.⁴ It should be trivalent after ad hoc hybridization. It shows variable covalency. In the trifluoride BF_3 it is trivalent. Boron hydrides show strange structures. The simplest is diborane B_2H_6 . It has the two hydrogen atoms located in the space between boron atoms. One hydrogen atom is above the plane of the rest of the molecule and the other is below the plane. A new bond type is introduced here - "two electron three center bond" A normal chemical bond is a two-electron two-center bond. Crystalline Boron is worse. It is one of the hardest materials known. It contains Boron icosahedra that cannot be visualized on the aufbau atom.

We may sum up the ad hoc assumptions in the application of QM to Chemistry: hybridization, σ -donation- π -back-donation bond, and two-electron-three-center bond.

3.4 Oxygen paramagnetism

Molecular oxygen shows paramagnetism⁹. This was described as a prediction of the Molecular Orbital method and was considered to validate the procedure. Oxygen molecule would have a plane of symmetry across which all moments should cancel out. This plane has to be a chiral plane in molecular oxygen for moments do not cancel out across a chiral plane. They retain their opposite sense like the poles of a magnet. A chiral plane means structure at the atomic level in oxygen. Such a structure is not allowed in QM. This 'structure' is

responsible for antiferromagnetism displayed by FeO and MnO. The moments acquire opposite sense across a chiral plane mediated by oxygen.

Magnetism is also a chiral phenomenon. The model for the iron $^{26}\text{Fe}_{56}$, based on the assumptions of the Unitary Model atom is made up of two chiral halves that account for the two poles of the ferromagnet.

3.5 Anthracene linear dichroism

Crystalline anthracene shows linear dichroism ¹⁰, an indication of dissymmetry in a molecule that looks perfectly symmetrical. Linear dichroism is correctly described as anisotropy in the absorption of polarized light. We had drawn attention to the possibility of q-surface fixation in our comments on anthracene electron density diagram. Q-Surface fixation is responsible for the linear dichroism of anthracene that cannot be accounted for by the QM.

4. Electric Current and magnetism ^{5, 11}

(23 February 09)

Magnetism and electricity are related phenomena. Magnetism is capable of transmission through space whereas electricity would need a medium for transmission.

We shall consider electricity first.

The characteristics of electricity are as follows:

It needs the medium of a conductor for transmission. It does not pass through space.

Its speed had not been measured but it appears to be high comparable to that of light. It would need enormous energy to accelerate the electron, a particle with mass, to such high speeds.

The voltage is the driving force for the flow of electricity. The speed is however independent of the voltage. High voltage current and battery-based current (12v)

used in copper cable telephony travel at the same apparent speed. These two facts would preclude any particle with mass like the electron as the carrier of electricity.

Electric current should therefore necessarily be considered a vector field carrying 'charge'. That it is a helical field follows from the fact that the current flowing through a conductor penetrates only a few atoms deep below the surface. Any other configuration for the current like the wave would require deeper penetration. The carbon nano tubes obtained by sparking at graphite electrodes have aromatic rings arranged in a helical fashion. The last important fact is that alternating current has two halves. Their individuality could be explained only in terms of chiral helical fields for the two parts of the AC.

It is known that a positron and an electron annihilate each other. While energy helices may form double helices without annihilating each other the charge vector helices may annihilate each other giving rise to photons. There is therefore no possibility of formation of a double helix with unlike charge vector helices.

Since like charges repel each other there would be no double helix corresponding to dark energy.

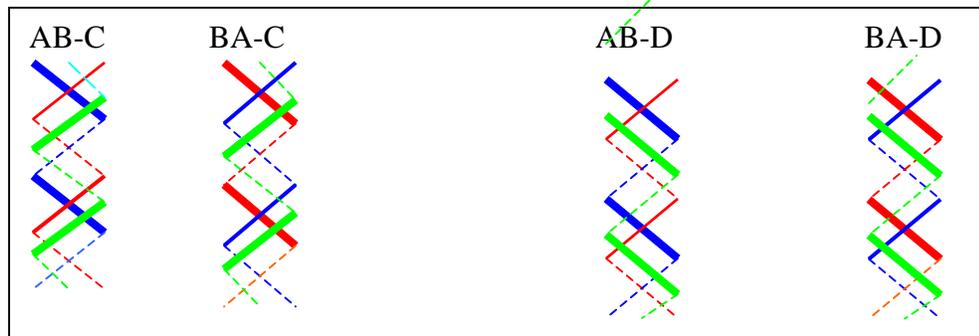
Magnetic fields travel through space. Unlike light they do not travel in straight lines with no specific target. They travel from one magnetic pole to the opposite pole. We have seen such charge vector fields cannot form double helices with both like and unlike helices. Magnetism then is a charge vector field formed by a single helix riding on some medium. Low frequency radiation with a double helical structure would be ideal for this purpose. Radiation provides the 'piggy back' for the charge vector to ride upon. In this view there are four possibilities for the charge vector to form a three-stranded helix with radiation.

If the chiral double helices of radiation are designated AB and BA (red and blue lines) and the chiral helices of opposite electric charges are designated C and D (greenish yellow) there are four possibilities in which the charge helices might form a three-stranded helix with radiation. These are AB-C, AB-D; BA-C and BA-D.

If AB-C and BA-C would designate, say, the North Pole and AB-D and BA-D should designate the South Pole of a magnet. The magnetic field lines between the two poles are represented by these two combinations. These two combinations, {AB-C: BA-C} and {AB-D: BA-D} are also present in the magnetic fields in outer space.

The charge vectors C and D determine the character of the field. The radiation that carries these vectors does not make any contribution. We had pointed out that light would flow in the same direction even in chiral (non super imposable) mirror image universes. This is because the double helix radiation vector (AB-BA) is identical with its mirror image.

(AB-BA || AB-BA)



Radiation helices- Blue and red lines; Charge vector helix yellowish green.

5. Inert Gases, superconductivity and Meissner effect^{5, 12} (Beiser 2004, Scurlock 1992)

Under Beryllium we had argued that Argon should not behave like an inert gas since it has unfilled electron shells. We prefer the alternate assumption that there are no extra-nuclear electrons in inert gases. The spectra are observed under high-energy excitation of the atoms. We examine below the implications of our assumption.

5.1 Liquid Helium^{12, 13}

As we said earlier the inert gases do not have any extra-nuclear electrons. Helium falls in this category. Inter-atomic attraction must be nil in the gas and accounts for its highest atomic volume for any element. Even the so-called 'volume' is due to gravity and not due to weak attractions between atoms. Liquefaction of helium means that the atoms of Helium had lost all their kinetic energy and settled under gravity. This is He-I. Because there is no inter-atomic attraction the liquid has no surface tension or viscosity. It is not a liquid in the conventional sense but only a collection of atoms settled under gravity. It still has atoms vibrating about a mean position. Further cooling arrests even this pseudo motion to give He-II. There is no phase change in going over from He-I to He-II. Gravity would continue to pull these atoms downwards. In response to this force a mono-atomic layer would move upwards along the walls of the vessel and flow over in a siphoning action. Thus all the properties of Liquid Helium are explained without invoking super-fluid or a special state of matter.

5.2 Meissner effect and superconductivity

Meissner effect is the disappearance of magnetic properties under superconducting conditions.⁵ (Beiser, 2004) The two effects are related. As we had seen in Helium, in extreme cold complete electron or charge subsidence takes place. In superconducting systems the electron subsidence is full and complete. We may now define the conditions anticipated for superconductivity. There should be continuous contact at the molecular or atomic level in the superconducting state. The electron or charge subsidence should be complete. The metallic state provides for continuous contact. Even here metals with 'closed

shells' like Lead, have an advantage in that they start with a partly electron or charge subsided state. But metallic state is not an imperative condition. Some mixed oxides have been found to serve the purpose. ¹³ (Vidali 1993) The electronegativity of oxygen serves to make charge subsidence easier. We had noted the subsidence effect of fluorine atoms in binary compounds. It is not surprising that Boron Nitride has a high super-conducting temperature. The ideal system would be a fluorine-containing metallic polymer like a continuous thread of teflon.

6. Cold fusion ¹⁴

Electron or charge subsidence provides a simple explanation for the nuclear fusion at near room temperatures observed by Taleyarkhan and his colleagues under conditions of bubble collapse. The conventional explanation preferred by the authors is that bubble collapse creates immense pressures of the order of a few million atmospheres and similar high temperatures. This assumption violates common sense. A simpler alternative is the assumption of charge subsidence. The first step is the generation of low energy deuterium radicals by the sonar fission of carbon deuterium bond. It would be facilitated by the presence of the adjacent keto group in the deuterated acetone. Alternatively the deuterium atoms may arise from the enol form of the deuterated acetone. Complete fission is not absolutely necessary for the purpose. Charge subsidence on the D-atom then takes place to give a dineutron. ¹⁵ One would expect the subsidence to be more facile at lower temperatures. This is indeed found to be the case. Fusion is observed only close to 0° C. Bubble collapse brings the neutral deuterium atoms or dineutrons within the range of strong nuclear force. Fusion under these conditions is automatic. The probability of the particles being brought within the range of the strong force is of course very low. Consequently the fusion observed is not much. A few million atoms fuse over 12 hours. This would work out to a miniscule 10^{-18} gm. Moles. A corollary is that the Coulomb repulsion is an over-rated obstruction for fusion. Fusion at ordinary temperatures is known even for

heavier atoms like lead (atomic number 82) and chromium (atomic number 24)
⁴(Greenwood 1997) which fuse to give Seaborgium (atomic number 106).

7. Proton sites and nuclear structure

Nearly 100 years have passed since the discovery of the atomic nucleus. In spite of all efforts we are nowhere near an acceptable view of the structure of the nucleus. ^{15, 16, 17}

We have assumed that the nucleus has protons and neutrons but we have no idea about their location. The simple idea that the covalent bonding sites might be proton sites had not been considered. It is also more easily understood that proton or charge sites in the nucleus may all be located on the periphery or the outer surface of the nucleus. In the case of covalence of Carbon, the tetrahedral carbon survives in all the bonding patterns. Further the swinging olefinic bond, that we find in Zeise's salt, raised the question of the permanence of electrons in the atom. We have adduced evidence that electron count is variable depending upon the bonding pattern. Additional chemical evidence also indicates that the electrons or charges may rise and subside as the context demands. Because of the survival of the tetrahedral structure in all bonding contexts in carbon, there is no chance for probability about the behavior of electrons. This is the fundamental conflict between our model and QM. A wider debate is called for.

8. Central dogma

The assumption that underlies the quantum model is that the nucleus acts as a point charge holding the electrons within the atom and does not have any influence on the behavior of electrons ^{1b} Whatever the validity of the idea in other areas we find that it is not valid for chemical systems. We have indicated that this might be because in chemistry we deal with individuality that cannot be subject to probability considerations. Thus the entire area of quantum mechanics is open to debate. The late J.T.Cushing in his book ¹⁸ on the origins of the probability says the idea was accepted due to a 'social contingency' because scientists did not want to leave the field open to doctors of divinity. This is unfortunate. We are

facing the consequences of the regressive notion that lacked the objectivity required of scientists.

REFERENCES:

1. a. For quantum mechanical concepts and definitions see Quanta, A handbook of concepts, P. W. Atkins, OUP, 1991; b. For a general discussion of atomic structure see E. U. Condon and H. Odishaw, Handbook of Physics, sec7, McGrawHill , 1967
2. a. R. G. Woolley, J.Amer.Chem.Soc. 1978,100,1073; b. S. J. Weininger, J.Chem.Ed., 1984,61,939.
3. D.M.P. Mingos, Essential trends in Inorganic Chemistry, OUP, 1998;
4. N. N. Greenwood and A. Earnshaw, Chemistry of the Elements, Butterworth, 1997
5. Arthur Beiser, Concepts of Modern Physics, Tata-McGrawHill,2004;
6. N. A. Dyson, X-rays in atomic and nuclear physics, 2 Ed. Cambridge Univ. Press 1990.
7. R. Hartley, Angew.Chem.Int.Ed. 1972,11,596
8. K. B. Wiberg, Accs.Chem.Res., 1984,17,379
9. K. M. Mackay, R. A. Mackay, W. Henderson, Introduction to Modern Inorganic Chemistry, Hamilton NZ 1995
10. Alison Rodger and Bengt Norden, Circular dichroism and linear dichroism OUP 1997.
11. S. Rama Reddy Electromagnetic theory, Scitech, 2002.
12. Monographs on cryogenics Oxford science publications; History and origins of cryogenics, Ed. Ralph G. Scurlock 1992- Part VIII
13. Superconductivity : the next revolution. Gianfranco Vidali 1993; Super conductors, the breakthrough: Robert M Hazen
14. R. P. Taleyarkhan et. al. Science, 295, 1868, 2002

