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Research Article

Keywords: orbital angular momentum, s electron occupancy, dimension of angle, quantum technology, quantum computer, qubits.

Posted Date: March 3rd, 2021

DOI: <https://doi.org/10.21203/rs.3.rs-247788/v1>

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Probing the private quantum life of s electrons in atoms of Nanomaterials -A new quantum theoretical insight

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Abstract

The exotic properties exhibited by some of the nanomaterials could not be explained by the existing quantum theory. As a result one is forced to look back at the development of the quantum theory and some of the inelegancies. First, the quantized orbital angular momentum of s electron in an atom is taken as zero. This may be an acceptable fact for s electrons in an individual atom, but for the s electrons in a crystal or nanomaterial, this is far from the real situation. Secondly, in the wave function $\Psi(r,\theta)$, θ is considered as a dimensionless variable. These inelegancies lead to the impression that the present quantum theory is a steppingstone to a more complete description of nature. Here arises a necessity for probing the private quantum life of s electrons in crystal or nanomaterial. By assigning dimension to θ on par with r , we have quantum engineered the orbital angular momentum and hence the orbital degrees of freedom of s electrons and their signatures in a crystal. This restoration leads to new non-zero angular quantum numbers to s electrons of atoms in a crystal/nanomaterial. As a result the s electron occupation in nanomaterial is altered. Its new physics implications in material science, quantum chemistry and quantum technology are highlighted in this paper.

Keywords: orbital angular momentum, s electron occupancy, dimension of angle, quantum technology, quantum computer, qubits.

1. Introduction

Quantum mechanics developed during the last century is considered as a unique modern theory. This led to the scientific and technological advancements which completely changed lifestyle of humanity. This is called the quantum revolution 1.0 and we are in the beginning of quantum revolution 2.0. Currently many new materials exhibit exotic properties like, unconventional superconductivity [1,2], room temperature superconductivity [3-5], reduced magnetism [6,7], reduced Pauli repulsion [8], giant negative thermal expansion [9] and unconventional ferroelectricity [10]. These exotic properties could not be explained completely

with the existing quantum mechanical theory which is mysterious yet incredibly accurate. But in some aspects it looks incomplete. One of them is the dimension of angle, θ . In the development of quantum theory r and θ played equal role but θ is not given its due place because of its dimensionless nature. Scientists attempted [11] to consider angle as a fundamental entity along with Length (L), Mass (M) and Time (T). Also there were attempts to assign dimension to angle [12,13]. But there is no reference to quantum theory where θ plays important role along with r . In a recent paper we have assigned dimension to angle [14] and it is found to be “curvature” denoted by C . This angular “curvature” is a measure of the amount of bending of the segment of the curve/surface. Another one is the quantized orbital angular momentum of s electron, whose average value is taken as zero. This may be justified for the s electrons in an individual atom, from the measurement point of view. But for the s electrons in a crystal/nanomaterial this may not be true. So far nobody has peered into the private quantum life of s electrons in a crystal/nanomaterial. In this paper we probe the quantum state of these s electrons under a new environment where angle has dimension. We have deduced the quantized orbital angular momentum of the s electron for the first time using quantum engineering.

2. Quantum engineering the orbital angular momentum of s electrons

2.1. Missed orbital angular momentum of s electrons in crystal

In the present quantum mechanical theory the quantized orbital angular momentum of s electron in an atom is zero ($\ell=0$). With this theory experts could explain most of the phenomenon in atomic and condensed matter physics. But in recent times exotic properties are exhibited by new materials, especially by nanomaterials, which could not be explained using the present quantum theory. This situation warrants one to peep into the private quantum life of s electrons in crystal, whose quantized orbital angular momentum is considered as zero so far. In physics no entity is zero. Let us have a close look at the angular momentum states of the electrons in an atom. The different angular momentum states are more about how different quantum phases are embedded in the wavefunctions, with a measurable outcome. May be in atoms this s electron orbital contribution is not measurable, but in condense matter (especially in nanomaterials) this s electron orbital contribution might be measurable. The electron dynamics in the condensed matter is entirely different from that of the atoms. These s electrons might have non-zero orbital angular momentum like the other p , d , and f electrons. With $\ell=0$, we have missed

the orbital angular momentum and the important signature corresponding to the orbital angular momentum of the s electrons, the orbital degrees of freedom, in crystal. We quantum engineered, using the newly introduced dimension of angle, and consequently restored of orbital angular momentum of the s electrons in crystal/nanomaterial as detailed below.

2.2. Uncertainty relations and commutation relations

The important and popular uncertainty relations are [15]:

$$\begin{aligned}\Delta x \cdot \Delta p_x &\geq \hbar \\ \Delta \phi \cdot \Delta J_z &\geq \hbar \\ \Delta t \cdot \Delta E &\geq \hbar\end{aligned}\quad (1)$$

All the quantities involved in the above uncertainty relations do have dimension except the angle (ϕ). Like other quantities in the above relations angle (ϕ) also should have dimension and it is found that “curvature” is the dimension of angle denoted by the letter C [14] as pointed out already.

Orbital angular momentum plays important role in electron dynamics. The quantized orbital angular momentum is defined by the commutation relations [15,16] of the angular momentum operators L_x, L_y, L_z ;

$$[L_x, L_y] = i\hbar L_z ; [L_y, L_z] = i\hbar L_x ; [L_z, L_x] = i\hbar L_y \quad (2)$$

$$[L^2, L_x] = [L^2, L_y] = [L^2, L_z] = 0. \quad (3)$$

These commutation relations arise from the above uncertainty relations which can be expressed in the form,

$$[x, p_x] = i\hbar ; [y, p_y] = i\hbar ; [z, p_z] = i\hbar \text{ and } [\phi, L_z] = i\hbar. \quad (4)$$

The new relation $[\phi, L_z] = i\hbar$ implies that the angular position ϕ and related angular momentum in the perpendicular direction L_z cannot be determined simultaneously with a high degree of accuracy. This means that ϕ and L_z are canonically conjugate variables similar to x, p_x ; y, p_y ; z, p_z and E, t . Now all of them including ϕ are having dimension. From the relation $[\phi, L_z] = i\hbar$, one can write the commutation relation between the operators corresponding to angle, O_ϕ and angular momentum operator L_z as,

$$[O_\phi, L_z] = i\hbar L_\phi. \quad (5)$$

where L_ϕ will take suitable form depending upon the nature of operator O_ϕ . Here we can associate the rotation operator [17] with angular operator O_ϕ . Now the

lowest order rotation (about z axis) operator corresponding to the angular operator O_ϕ turns out to be the Pauli operator σ_z . Also for the s electron the lowest order of orbital angular momentum operator is the spin angular momentum operator σ . So O_ϕ and L_ϕ take the form of the spin operator and we will have the following commutation relations:

$$[\sigma_x, \sigma_y] = i\hbar\sigma_z ; [\sigma_y, \sigma_z] = i\hbar\sigma_x ; [\sigma_z, \sigma_x] = i\hbar\sigma_y \quad (6)$$

Where σ_x , σ_y and σ_z are Pauli matrices. Through this formalism one can restore the orbital degrees of freedom and hence the orbital angular momentum of s electrons in the atom.

2.3. Restoration of orbital angular momentum of the s electrons

With the above commutation relations (Eqns.2-6), we are now in a position to restore the orbital angular momentum of the s electrons, which is zero in the present quantum theory. Comparing the relation $[O_\phi, L_z] = i\hbar L_\phi$ with commutation relations (Eqns.2 and 6) one can infer that O_ϕ will have degrees of freedom similar to that of the orbital degrees of freedom of L_z (due to the angular momentum). From the commutation relation between angular operator O_ϕ and angular momentum operator L_z , the orbital angular momentum quantum number of the s electron (call it ℓ') turns out to be the same as spin angular momentum, $\ell' = 1/2$. Now, for the s electrons of the crystal, the orbital angular momentum takes its lowest value equal to the spin angular momentum, but like spin it is not an inherent property. Thus the quantized orbital angular momentum of s electron is estimated as $\ell'(\ell'+1)\hbar^2 = 0.75\hbar^2$. Here, now the new quantum number is $\ell' (= 1/2)$ and the corresponding z (magnetic) quantum numbers are $m_{\ell'} = 1/2$ (clockwise) and $m_{\ell'} = -1/2$ (anti-clockwise).

Thus through angle with the newly found dimension, the orbital degrees of freedom and hence the corresponding new quantum states of the s electrons of the atom in the crystal are restored. The related quantized orbital angular momentum of s electron in the crystal may be measurable now. In addition to the spin states (spin up, $m_{s'} = 1/2$ and spin down, $m_{s'} = -1/2$), the s electrons can have states corresponding to the orbital degrees of freedom ($m_{\ell'} = 1/2$; $m_{\ell'} = -1/2$). In a crystal/nanomaterial, in the s shell of the atom, now it is possible to accommodate 4 electrons, s^4 . For p, d, f electrons the orbital degrees of freedom are already taken into account through the non-zero values of ℓ and there is no change in the occupation number of these shells. Additional degrees of freedom due to the orbital angular momentum of the s electrons of the atom will not have any effect on the spectra of molecules and atoms

. May be in atoms this s electron orbital contribution is not significant and not measurable. But in condensed matter (specially in nanomaterials) this s electron orbital contribution might be measurable. Thus there is a choice to have s electron occupancy more than 2. We have a flexibility of altering the number of electrons in the required s shells to account for the new avatar of modern materials. Now one can definitely announce that nature has provided more space in s shell than we thought, in atoms of the crystal/ nanomaterials.

3. Exotic properties

Unconventional Superconductivity in twisted bi-layer graphene [1], in cuprate and iron based system arises because of the complex interaction among the valence electrons. These exotic properties of nanomaterials can be explained, to some extent, with the help of the new flexible s electron occupation. Strong coupling between the spin and orbital degrees of freedom is vital in generating the exotic band structure of materials [2]. It is reported [3,5] that LaH_{10} and YH_{16} become superconducting under very high pressure range. Recently room-temperature superconductivity is observed in a carbonaceous sulphur hydride [4] under high pressure. In these materials s electrons play a major role. These s electrons undergo Fermi condensation (more than 2 electrons in the s states) due to the restoration of orbital degrees of freedom of s electrons. This induces Bose Einstein Condensation leading to superconductivity. This is similar to the phenomenon where in states occupied by more than two electrons are found in one-dimensional $LaAlO_3/SrTiO_3$ channels [18].

Reduced magnetism in Fe , Co , Ni [6,7] and in cuprates [19] and the unconventional ferroelectricity in moiré heterostructures [20] can be explained using the new flexible s electron role with non zero angular momentum. Michael addition reaction in chemistry is explained recently, after 130 years, by Hamlin *et al.*[8]. They reported that it is not because the orbital interactions and the electrostatic interaction get more stabilising, it is because the closed shell–closed shell Pauli repulsion becomes less repulsive. According to our proposed new flexible s electron occupation the s shells are no longer closed and the closed shell–closed shell Pauli repulsion becomes less repulsive because they are not actually closed.

4. Resonating Valence States (RVS)

Carbon is the only element which has the maximum number of allotropes. Pristine carbon comes in several forms. The different forms of carbon are diamond,

graphite, fullerene, nanotube, and single-atom-thick graphene. Carbon has a unique property of forming chemical bonds with itself leading to different structures. *sp*-hybridization is the specialty of carbon. Apart from the above allotropes, carbon displays non *sp*-hybridised bonding. Carbon cubic crystals are predicted by Volz *et al.* [21] and Iyakutti *et al.* [22], where carbon valence is 6. In this case, according to the flexible *s* electron occupation, the carbon atom's electronic configuration now is either $1s^4 2s^2$ or $1s^2 2s^4$. In carbon ring C_{18} , Kaiser *et al.*[23] have observed alternating single and triple bonds. In a recent theoretical calculation [24], it is reported, from the bonding characters for C_6 , C_{12} , C_{16} , and C_{20} molecules, that carbon-carbon bonds of cyclo[n]carbon changed gradually from double bonds to alternating single and triple bonds with increasing *n* value. In these cases the acquired valence state of carbon may be $1s^2 2s^4 / 1s^4 2s^2$ resonating with $1s^2 2s^2 2p^2$ state [25].

5. Quantum Technology

In this new technological area, quantum computing, quantum sensors, quantum cryptography, quantum simulation, quantum metrology and quantum imaging are some of the practical applications being developed. These are based on quantum entanglement, quantum superposition, and quantum tunneling. In quantum computing there is a stiff competition for achieving quantum supremacy [26]. Scientists believe that it is going to be the era of quantum revolution 2.0. The proposed new dimension of angle and the restored orbital angular momentum of *s* electrons will contribute additional new important inputs to quantum technology in the coming years.

5.1 Entanglement and qudits

Entanglement is the inability of quantum mechanics to define two quantum systems independently after they interact and separate. When two *s* electrons (two quantum states) interact and separate, they are entangled through their spins. The pre-request for entanglement is the identification of quantum states, qubits, which are to be entangled. Then such quantum states can be encoded in various degrees of freedom of atoms. For example, qubits can be encoded in the degrees of freedom of electrons surrounding the atomic nucleus. Orbital angular momentum states are tried for high-dimensional quantum entanglement /communication by researchers in this field [27]. Having established the orbital angular momentum and the orbital degrees of freedom now it becomes possible to use *s* electron orbital angular

momentum states in an atom to build qudits, the qubits of higher order. Also for quantum entanglement, it is easier and less expensive to quantum engineer qdits with s electrons compared to p or d electrons. Huan Cao *et al.* [28] reported the first distribution of three-dimensional orbital angular momentum (OAM) entanglement via a 1-km-long few-mode optical fibre.

7. Summary

Probing the private quantum life of s electrons in crystals/nanomaterial has led to new physics possibilities. With the introduction of dimension to angle (θ), on par with r , we have shown that it adds strength to the existing quantum theory in which $\Psi(r, \theta)$ plays the central role. Through the dimension of angle the orbital degrees of freedom of s electrons in the crystal are restored leading to a modified and flexible s electron occupation resulting in a higher occupation (up to 4 electrons) of s shell. The quantized orbital angular momentum of s electron in crystal is estimated as $0.75\hbar^2$. It will be an additional tool to explain exotic/unconventional properties, which modern materials exhibit. Nature has provided more space in s shell of the atoms in solids than we think. At this juncture, it is worth mentioning about the important natural constant α , the fine structure constant. It is considered to be the ratio of the orbital speed of electron to the speed of light [29]. Is there a hidden dimension in nature that somehow fix the value of α ?. May be this is the reason that people are still measuring the value of α , the fine structure constant [30]. We believe, like θ , α also has a hidden dimension, since the dimension of orbital speed is not the same as the dimension of linear speed of light.

Now angle with dimension C can be added as the fifth fundamental entity, Angle (C), along with Length (L), Mass (M), Time (T), and Charge (Q). Every theory is based on certain postulates and its validity is restricted to situations where these postulates are applicable. Extending the proposed flexible electronic configuration model of the atom to the nuclear shell model, we can account for the neutron dripline reported recently [31].

Acknowledgments

The authors express their sincere thanks to the crew of CCMS of the Institute for Materials Research, Tohoku University for their continuous support and help in using the CRAY-XC50 supercomputing facilities. Author KI is thankful to SRM Supercomputer Center, SRM Institute of Science and Technology, for providing the computational facility. The author KI is thankful to Prof. V. Devanathan and Prof. Velusamy for fruitful discussions.

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