Introduction to quantum mechanics essay

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Introduction

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The wealth of information in atoms and molecules can be achieved from quantum mechanical studies of their structural as well as various physical and chemical properties. Based on quantum mechanics [1-7], large number of approximation methods has been developed over the years for the complete solutions of atomic and molecular systems. Now-a-days, the availability of the computer hardware and software has been increased enormously. In addition, a large number of suitable computational methodologies and algorithms have been developed over the years for solutions of realistic problems in different branches of physics/chemistry. Making the use of the power of the present generation computers as well as computational methodologies and algorithms, we can perform large scale research just by performing high level quantum mechanical computations as an alternate tool of experiment. These high level computations some time meet the requirement for realistic problems in different branches in physics, even in atomic and molecular physics. Many complex molecules like drugs are designed on computer in modern days. Such computational attempts are helpful to the experimentalists because with the help of the theoretical idea achieved form these computer simulations, they can perform the real synthesis of these complex molecules in laboratories without much difficulties. Sometimes, it may not be possible to synthesize certain molecular systems which are very much unstable or poisonous or explosive in nature. But then one can carry out theoretical calculations and

computations to explore their structure and various properties without handling them in reality. Because of the availability of the faster and cheaper computer hardware, as well as a variety of suitable algorithms, theoretical investigations of various physical and chemical properties of these molecules are now become less expensive and easier. It is well known to scientific community that modern-day atomic and molecular spectroscopic studies require very expensive spectrometers and other sophisticated instruments for getting results with desired accuracy. But one can carry out theoretical and computation based spectroscopic studies of even complicated atomic and molecular systems with utmost accuracy without taking any help of such kind of sophisticated and expensive instruments. Moreover, the interpretation and understanding of every experimental finding needs the knowledge of theoretical background. It is, therefore, essential to carry out theoretical studies beside each and every experiment, wherever possible, to ensure the validity of the experimental findings.

Classical mechanics [8] can explain accurately the dynamical features of the objects of relatively large mass and low velocities. But it is not sufficient to describe the interactions among subatomic particles of colliding galaxies. If the velocity of the object is comparable with that of light, one must use Einstein's relativistic mechanics in which the variation of mass with velocity has been taken into consideration. If the mass of the object is very small, the non relativistic quantum mechanics due to Heisenberg and Schrödinger is applicable. If the mass is very small but the velocity of the object is comparable with the velocity of light, one should use the relativistic quantum mechanics developed by Dirac [9]. Therefore, depending on the mass and

velocity of the object, one should employ the appropriate mechanics for determining its dynamical features.

The computations of large systems may, therefore, be carried out by using appropriate mechanics. Because of the advancement of the computer hardware and software technology, one can easily carry out these computations. Sometimes, huge computations may have to be performed in this connection. One has to solve 2nd order differential equations with several million variables. However, suitable techniques are available to reduce the size of the secular equations drastically at the cost of some accuracy and hence large-scale computations can be performed successfully.

The electronic structure and spectroscopic properties of atoms, molecules and solids can be determined from quantum mechanical solutions [10-14] of the systems. Atoms and molecules in the electronic structure theory are in stationary states. The time dependence of the wave function can thus be separated so that one needs to work only with time-independent solutions. Born-Oppenheimer approximation, which allows the nuclei to be in fixed co-ordinates during the motion of electrons, is usually employed for the calculation of the electronic structure of molecules. It is, therefore, possible to carry out calculations on specific molecules of physical and chemical interest with the aim of getting structural aspects and spectroscopic properties which otherwise may not be obtain from the experimental work. In many cases, the experimental data may be interpreted from the computational results.

The velocity of the interacting particles in lighter atoms and molecules is considered to be negligible compared to the velocity of light. So, one may not include the relativistic effects as they are negligibly small. But for the calculations of the heavier atoms and molecules, the relativistic corrections are needed and hence one must use the relativistic quantum chemistry [15-17]. It requires a modification of the non relativistic Hamiltonian with various relativistic correction terms such as mass-velocity correction, spin-orbit correction, Drawin correction, Breit interaction etc. Actually, after the discovery of the theory of special relativity, relativistic effects on the electronic spectra of atoms and molecules become very much important. The relativistic effects are prominent on the electronic spectra of those molecules / their ions for which the nuclear charges of the constituent atoms are large i. e. when atoms with high Z are present. So, in order to obtain accurate spectroscopic features of heavy or moderately heavy molecules / their ions, one must take the various relativistic effects into account in an efficient way. A number of algorithms have been developed in recent years in these connections along with enormous enhancement in computing power. Therefore, the challenge is to exploit these developments to perform the high level computation based theoretical researches work which becomes an alternative to the experimental physical chemical researches.

References

[1] L. Pauling, E. M. Wilson, Introduction to Quantum Mechanics, McGraw-Hill, 1935.

[2] H. Eyring, J. Walter, G. E. Kimball, Quantum Chemistry, Wiley, New York, 1944.

[3] J. P. Lowe, Quantum Chemistry , Academic Press, New York, 1978.

[4] D. A. Mcquarrie, Quantum Chemistry, University Science, Mill Valley Calif, 1983.

[5] P. W. Atkins, Molecular Quantum Mechanics, Oxford University Press, New York, 1983.

[6] F. L. Pillar, Elementary Quantum Chemistry, McGraw-Hill, New York, 1990.

[7] I. N. Levine, Quantum Chemistry, Printice-Hall, N. J. , 1991.

[8] H. Goldstein, Classical Mechanics, Addition-Wesley, Reading, Mass, 1950.

[9] P. A. M. Dirac, The Principles of Quantum Mechanics, Oxford University Press, Fourth Edition, Oxford, 1958.

[10] R. G. Parr, Quantum Theory of Moleculer Electronic Structure, Benjamin, New York, 1963.

[11] J. A. Pople, D. L. Beveridge, Approximate Molecular Orbital Theory, McGraw-Hill, New York, 1970.

[12] J. N. Murrell, A. J. Harget, Semiempirical Self-Consistent-Field Molecular Orbital Theories of Molecules, Wiley-Interscience, New York, 1971.

[13] R. S. Mulliken, W. C. Ermler, Diatomic Molecules, Academic Press, New York, 1977.

[14] R. S. Mulliken, W. C. Ermler, Polyatomic Molecules, Academic Press, New York, 1981.

[15] P. Pyykk *Ó§* , Relativistic Theory of Atoms and Molecules, Springer-Verlag, Berlin and New York, 1986.

[16] K. Balasubramanian, Relativistic Effects in Chemistry Part A. Theory and Techniques, Wiley-Interscience, New York, 1997.

[17] K. Balasubramanian, Relativistic Effects in Chemistry Part B. Applications to molecules and Clusters, Wiley-Interscience, New York, 1997.