Editorial*

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The June issue of *Resonance* features Clemens C. J. Roothaan—a Dutch *ingenieur*, turned into a physicist and chemist. Roothaan's career as a graduate student started in an unusual and traumatic environment during World War II. Because of his ethnic background, he had to spend almost the entire period of his graduate days in Nazi concentration camps. However, he managed to continue his studies with favorable assistance from his professors at the Technical University of Delft.

During the past months, the pandemic around the world has had the worst impact imaginable. While students are still pursuing academics during these difficult times, I hope the exposure to Roothaan's career brings additional inspiration to cope up with the current situation. Times have changed, and any piece of information is just a click away today, unlike in the days of Roothaan.

After graduation Roothaan emigrated to the United States and continued living there for the rest of this life. He joined as a PhD student in the research group of Robert Mulliken at the University of Chicago and later joined the Physics Department and also served as the Director of the University Computing Center.

Roothaan's PhD work evolved into a classic and appeared in the *Reviews of Modern Physics* in 1951—"New Developments in Molecular Orbital Theory". This work was based on the procedure developed by Douglas Hartree and Vladimir Fock in the late 1920s and early 1930s, called the 'self-consistent field' (SCF) method, to calculate the wave function and energy of many-electron systems by solving the time-independent Schrödinger equation from fundamental physical principles (*ab initio*). The approximation made in the theory was to write the many-electron Hamiltonian

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*Vol.26, No.6, DOI: <https://doi.org/10.1007/s12045-021-1175-3>

as a sum of one-electron Hamiltonians by treating the inter electronic interactions in an average way. The spin orbitals that appear in the many-electron wave function are optimized variationally to represent the electronic ground state of the system. The ansatz resulted in a nonlinear integro-differential equation—the ‘Hartree–Fock equation’—which was solved iteratively, but it was mathematically complicated for molecules.

Roothaan focused on this problem and made a seminal contribution to transforming the Hartree–Fock equation into a set of linear algebraic equations by introducing the concept of linear combination of atomic orbitals (LCAO) to represent molecular orbitals, which are solved by standard matrix algebra. Roothaan called this the ‘LCAO–SCF method’, which represents a milestone in the further development of molecular quantum chemistry. During his professional career at Chicago, he concentrated on the calculation of integrals that appear in the LCAO–SCF formalism in a systematic way and developed tools to translate them into computation.

The scientific career and work of Roothaan is documented in two articles in this issue. A brief chronological account is presented in the Article-in-a-Box and a more complete description is presented in the article by Shridhar R. Gadre and Subhas J. Chakravorty.

Apart from the articles noted above, there are other articles written by students and colleagues which makes this issue of *Resonance* interesting. There are three articles appearing in the Classroom section. The article by Jayanth Vysanaker and Rajaram Nityananda analyses the shortest path and configuration of a rubber band wrapped around a sweet box—an interesting study of closed curves on a cuboid. The article by Arvind Singh and Priyanka Chaturvedi illustrates the underlying assumptions made in the derivation of the error propagation equation and discusses its origin. The method to estimate error in nonlinear transcendental functions is also suggested by the authors. It is interesting to note that “error is not a mistake in science”. Venkata Karthik Bandaru suggested a schematic proof of graceful labeling of graphs that are called caterpillar trees.

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The analytic solution of second-order Airy differential equation, contour integration of Airy functions and their derivations using Fourier transformation relation is presented in a general article by M S Ramkarthik and Elizabeth Louis Pereira. Application of Airy functions in WKB method and quantum bouncing ball is discussed by the authors. Sameen Ahmed Khan illustrates how irrational numbers can be learned through basic trigonometry. In this context, the proof of Niven's and Paolillo–Vincenzi theorems is discussed. The irrationality of π and π^2 is proved, and Ram Murty and Kumar Murty theorem is revisited. It is noted that elementary trigonometry and basic calculus would cater to the needs of frontier research. The article by Indranil Ghosh in the general section discusses the application of quantum game theory and is a continuation of Part-I of the article written by him in an earlier issue of *Resonance*. The documentation of groups of cave animals found in the state of Meghalaya by Uttam Saikia and Manuel Ruedi is quite interesting. The variety of bats discovered there and a threat to their life due to coal and limestone mining that is causing topographical and ecological damage is an important information conveyed in the article. I hope the readers enjoy reading these articles.

Finally, I appreciate the hard work put in by R Pusphavathi and Geetha Sugumaran to bring out this issue on time, mostly working from home, in these difficult pandemic times.