

Editorial

K L Sebastian, Chief Editor

This issue of *Resonance* covers the life and work of the extraordinary Indian scientist, Aneesur Rahman. This is the fiftieth year of the publication of his seminal paper in *Physical Review* (**136**, A405, 1964). In it he performed the first molecular dynamics simulation of liquid argon, thus starting the new era of studying condensed phases by simulation. Since then, the area has grown enormously, thanks to the increased availability of computing power. His life and work are covered in an article written by Sen and Sastry. Rahman's work is characterised by the elegance of the methods that he chose. The work that always has a fascination for me is the study of an electron in molten KCl. This is a very difficult system to study, because the electron needs to be treated quantum mechanically while the potassium and chloride ions are heavy and classical mechanics is enough, and further the system is at high temperature. How does one handle all these? The very elegant answer that Parrinello and Rahman (*Journal of Chemical Physics*, **80**, 860, 1984) came up with was to use the Feynman path integral approach to simulate the electron – this enabled them to map the behaviour of the electron into that of a long molecule, obeying the equations of classical physics. Thus all that one had to simulate was the classical dynamics of a single long chain molecule trapped in molten KCl. The study showed that the electron is trapped in an F centre. Rahman's work has had a great impact on the area and people working in this area like to believe that he would have won the Nobel Prize if he had lived longer.



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Resonance had featured the Italian physicist Enrico Fermi in the January issue. The article by Amit Roy in this issue covers another major aspect of Fermi – his outstanding abilities as an experimentalist which won him the Nobel Prize in Physics. This issue has an interesting Classroom article by Das and Kumar, who discuss unusual aspects of a very simple problem – the dynamics of coupled harmonic oscillators. Deb discusses the application of variational Monte Carlo method to quantum problems, while Rao and Ramakrishna discuss embedding of a semigroup in a group. Yet another interesting article is the one on skinks of the Western Ghats by Datta-Roy.

