TIFR Centre for Interdisciplinary Sciences, Narsingi, Hyderabad 500075

Seminar

Application of the Finite Element Method to Quantum Mechanics

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The finite element method (FEM) has been used in the design of airplanes, and bridges and dams across rivers. Its successes can be traced to the fact that FEM may be thought of as the discretization of the action integral prior to the application of the principle of least action. This implies that the method can be applied fairly universally to solve physical problems.

I will briefly describe the method and show how this can be used in solving quantum mechanical problems.

- The standard 1D example of the radial equation for the hydrogen atom will be used to illustrate the basics.
- The hydrogen atom in a magnetic field has a Schrödinger equation that is non-separable; the FEM has been used to obtain eigenvalues accurate to 1 part in 10^6.
- Quantum mechanical tunneling and scattering can be cast in the form of a variational problem, and again all the power of the FEM can be brought to bear on such complex calculations.
- The connection with the action provides a unique way of improving the mesh for discretization of the physical region, allowing us to employ computational resources in the most economical manner.
- Quantum semiconductor heterostructures provide new opportunities to investigate fundamental quantum mechanical effects while holding forth the promise of new optoelectronic devices. The design of quantum well laser operating in the mid-IR (2-6 microns) and the TeraHertz (70-200 microns) regions of the spectrum will be mentioned to illustrate how the FEM has permitted the novel paradigm of "wavefunction engineering" to come into its own. The conserved current continuity conditions at interfaces are determined by a gauge-variational method and the optical matrix elements are obtained through the Feynman-Hellmann theorem.
- Square quantum wires with finite barriers give rise to confined states in a non-separable potential. The spectrum shows a remarkable removal of "accidental degeneracy" associated with the 2D infinite quantum well system.
- Quantum waveguides and scattering centers in them, and 2D open domain scattering are recent problems of interest in the context of novel aspects quantum transport.

These examples will be used to emphasize aspects of FEM, and demonstrate the flexibility, the power and the generality of the FEM, and its use in nanoscience.

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11:30 AM (Tea/Coffee at 11:15 PM)

Seminar Hall, TCIS