Hevesy György PHD School of Chemistry, ELTE Faculty of Science
SELECTED METHODS OF MODERN QUANTUM CHEMISTRY, Kém/255.
Dr. Gábor Pongor

INTRODUCTION

Vectors and vector fields. The history of the ”nabla”. Postulates of the classical and the non-relativistic quantum mechanics. The atomic units. The principles of mechanics (Lagrangian, Hamiltonian). Special relativity theory. The Maxwell equations. Baron Eötvös and Maxwell. The simplification of Heaviside. The CGS and SI units in mechanics and electrodynamics. Electric and magnetic forces using Lagrangian and Hamiltonian formalism. The Lorentz-Heaviside force. The Hamiltonian equation of motion.

CONSERVATIVE FORCES AND THE LORENTZ-HEAVISIDE FORCE

Simple, informal definition. Path independence. Mathematical description (three equivalent conditions). Conservative and non-conservative forces. Is the Lorentz-Heaviside force conservative?

MAGNETIC RESONANCES

Magnetic susceptibilities. Electron in a homogenous, static and an oscillating magnetic field. The Bloch equations. Electron-coupled spin-spin interactions. Electron spin resonance. Nuclear spin resonance. The role of gauge-transformation. The gauge of potentials. The Coulomb-gauge. The Lorentz-gauge. The gauge-transformation and gauge-invariance in quantum mechanics.

THE AHARONOV-BOHM EFFECT

The assumption of Ehrenberg and Siday. The Bohm-paradox. The Aharonov-Bohm effect. Pure and mixed states, density matrices. Open, closed and isolated systems in quantum mechanics.

THE LONDON ORBITALS (LTO) IN QUANTUM CHEMISTRY

Form of the London-orbitals. Gauge invariant/gauge including orbitals. Lorentz and Hameka. The use of LTO-s in quantum chemistry. Ditchfield’s paper (perturbation theory). The method of Pulay and Wolinsky.