Preface

The objective of the present monograph is to propose a new probabilistic model in quantum mechanics where the probability wave functions of the quantum systems are obtained as solutions of the variational principle of minimum mean deviation from statistical equilibrium and independence where the values of the variational parameters involved are determined looking for stationary points of the mean energy of the system.

Part I deals with the general model and its applications to the standard systems (one or two particles in a box, the harmonic oscillator, and the hydrogen atom) without using the corresponding Schrödinger equations, and to the ground state of the helium atom for which there are excellent trial functions proposed in the literature, based on different variational methods. It also deals with a simplified model of the lithium atom which shows the necessity of taking the shell structure of more complex atoms into account.

Part II deals with the linear approximation of the probability wave functions induced by the minimum mean deviation from statistical equilibrium which is applied to the study of the structure of more complex atoms (the lithium, beryllium, boron, carbon, nitrogen, and argon atoms) in the ground state. The new tool allows us to calculate different correlations between electrons, the degree of stability of systems of electrons, and the amount of interdependence among different subsystems of electrons inside the atom.

The effective implementation of the formulas obtained is based on the software package MATHEMATICA which does both numerical computations and symbolic mathematics as well. Detailed computer programs are given at the end of each of the two parts.

Part I is more theoretical and is meant mainly for physicists and those interested in mathematical physics. Part II is more applied and is meant mainly for those working in quantum chemistry. The equations are numbered independently in the two parts of the volume. Each part is selfcontained and the prerequisites are kept to a minimum.