Numerical methods for electronic simulations

1. Introduction.

2. A bit of probability theory. 6

3. Classical Monte Carlo 6

4. Classical Langevin molecular dynamics at finite temperature 6

5. Hartree and Hartree-Fock approximation. 6

6. Correlation effects: Exact diagonalization. 6

7. Correlated wave functions and Variational Quantum Monte Carlo. 9

8. Diffusion Monte Carlo for bosons. 9

9. Finite temperature Monte Carlo, path integral 6

10. Quantum Monte Carlo by auxiliary fields. 6

At the end of this basic material, some of the following advanced recent numerical techniques will be discussed:

1. Fixed node approximation:
an approximate solution to the fermion sign problem instability.

2. Density matrix numerical renormalization group.

3. Optimization of correlated variational wave functions

4. Reptation Monte Carlo.

5. Worm algorithm for Path Integral Monte Carlo.