Study of Statistical Systems Using Monte Carlo Methods

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It is of prime interest in various fields to study a system which constitute of very large number of particles. The physical properties of such a system cannot be deduced by solving the classical Newton Laws (or Schrodinger Equation for quantum systems) sheerly because of the complexity and the very large number of equations and even larger initial conditions. For this statistical methods become an indispensible tool .In statistical approach towards the problem, it is of immense interest to find the partition function from which other expectation values of observables can be easily calculated .Since partition function cannot be calculated analytically except for few special and approximated systems ,computational methods have to be used to investigate the properties of the system.

Ising model in three dimensions is an analytically unsolved problem and the properties are studied using computational techniques. Monte Carlo methods are extensively used as an effective way to study these system. The basic idea behind this method is to simulate the system to its equlibrium condition and find the corresponding transition rates between the different states of the system ,such that the distribution is boltzmann . The expectation values of the observables then can be eventually evaluated in a straightforward manner.

This methodology is advantageous as we skip the task of summing over all states which is improbable for most of the system in consideration .In the thermodynamic limit there are effectively infinite number of states which all need to be sum up for an exact value of the partition function. However using this methodology we just need to sum up over the finite number of states the system goes through in the simulation .However, this induces errors in the

calculation as some of the states have not been taken into consideration .

I will like to investigate for efficient ways to model the system using computational techniques so that better estimate of the system observables can be made. Since computational cost is an important factor , I will like to carry out optimization study of the model. Also as it is important to estimate the error due to computational limitations so that difference between experimental observation and theoretical prediction can be accounted on that rather than on the theory , I will like to carry out the error analysis of the model.