ABSTRACT

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Thesis Title	**: Quantum Spin Model in Condensed Matter Physics and its Application to some Magnetic Materials.**

It has become possible to provide the description of macroscopic phenomena based on the understanding of mechanism occurring at the microscopic level. So, aim of condensed matter physicists is to determine the magnetic properties of material from mathematical models capturing the dominant interactions between the spins. Some of these models are analytically and exactly solvable but in most of the cases, even approximate analytic solution is a extremely complicated. So, numerical technique has become one of the powerful tool in condensed matter physics. We have written a code for exact diagonalization in FORTRAN 95 using Davidson's algorithm for iterative diagonalization which can calculate zero as well as finite temperature properties of magnetic systems. One of the biggest problem we encounter in exact diagonalization is dimensionality of the Hamiltonian matrix to be diagonalized. Dimensionality of the Hilbert space increases exponentially with the increase in number of spins. So, one is supposed to use various kind of lattice symmetries to handle the bigger lattice in order to explain the experimental realizations through model calculation. Here, we have used rotational symmetry because the Heisenberg Hamiltonian is rotationally invariant in spin space and hence total spin (S^{total}) is a good quantum number. We diagonalize the Hamiltonian matrix in $M_s^{total} = 0$ subspace for even numbered spin system(and $M_s^{total} = 1/2$ subspace for odd numbered spin-system) where M_s^{total} is the magnetic quantum number on which all the possible spins of the system can be projected. Our exact diagonalization code can calculate the ground state & few low lying excited states and their corresponding eigenvalues of a spin-system. Using these eigenstates and eigenvalues, we numerically calculate physical quantities like spin-gap, spin-spin correlation, static spin structure factor, partition function, magnetic specific heat, entropy and magnetic susceptibility of a spin-system.

First problem we have addressed is to reconcile the issue with dimensionality of $X_2Cu(PO_4)_2$,

where X= Sr, Ba. We performed exact diagonalization calculation and calculated zero temperature properties like spin-spin correlation, spin-gap and finite temperature properties like magnetic specific heat and magnetic susceptibility to show the effect of intra-chain and inter-chain couplings and observed that effect of inter-chain couplings on the physical properties of the system is negligible *i.e.* $X_2Cu(PO_4)_2$ is a one-dimensional material indeed.

In case of $J_1 - J_2$ model on square lattice, it is well accepted that the system has Néel ordering and collinear ordering for $J_2/J_1 \leq 0.4$ and $J_2/J_1 \geq 0.6$ regime respectively. In the intervening regime of frustration parameter, J_2/J_1, system has a quantum mechanically disordered phase or quantum paramagnetic phase. However, in real situation, materials like cuprate-superconductor have multi-layered structure of magnetic ions like Cu^{+2}. So, its a valid question to ask that what happens when inter-layer coupling is taken into account? This question is our second problem, we performed exact diagonalization calculation on a two-layered cluster of spins, calculated zero as well as finite temperature properties of the model. Exact diagonalization results infer that as we introduce interlayer couplings, the intermediate quantum paramagnetic regime tends to vanish and the critical value of interlayer coupling is 0.3 times the in-plane first neighbor coupling which is in agreement with the existing results.

Earlier, it was proved that ground state of a Majumdar-Ghosh chain can be obtained from a building block of three spins ($\mathcal{B}_3$). Further, one can question that does $\mathcal{B}_3$ captures the thermodynamic properties of whole chain? We calculate thermodynamic properties of the block and examine up to what degree it matches with the thermodynamic properties of the whole chain. We extended the idea of $\mathcal{B}_3$ in 2D and constructed a block of five spins $\mathcal{B}_5$ which is treated as a building block of 2D square lattice. We calculate zero as well as finite temperature properties of $\mathcal{B}_5$ and compare it with the experimental results of real materials. We find that properties of $\mathcal{B}_5$ qualitatively matches with physical properties of real materials, so, we can conclude $\mathcal{B}_5$ could be indeed a building block of 2D square lattice which captures some feature of infinite lattice.

Our last problem is related with quantum computation. A quantum computer must have quantum memory device, *i.e.* evolution of state of the quantum memory device should take place according to the laws of quantum mechanics and can be controlled. This controlled evolution of state of quantum memory device is called controlled switching. Here, we provide a scheme for controlled switching of a three spins-1/2 system with antiferromagnetic exchange couplings. We apply magnetic pulse to the system for a short duration, put some restrictions to the pulse to get any arbitrary superposition of states. This fulfills the rquirement of Grover's algorithm to make a quantum memory device. Hence our scheme may be used to make quantum memory device.