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Thesis title : **Exact Diagonalization studies on few electron Quantum Dots**

ABSTRACT

The work reported in this thesis is on the study of interacting mesoscopic systems consisting of double quantum dots. The study is important for both experimental and theoretical point of view due to their use in many areas of science and technology. The correlations leading to various phenomena in these systems can be studied in a controlled manner when double quantum dot systems are connected to the electron source and drain leads. The properties of the double quantum dot system can then be studied by varying any of the system parameters such as the dot energies, dot-lead couplings, interdot tunneling matrix-element, ondot and interdot Coulomb interactions etc. with respect to the chemical potential in the leads. The connecting leads can be the metallic ideal leads having flat-band structure or any arbitrary structure such as the single-walled carbon nanotubes. The double quantum dots in T-shaped geometry with these two different types of leads are considered. In the other part of the study ideal leads treated in zero-bandwidth limit are considered.

In the beginning, the double quantum dot based mesoscopic systems and interest in this area of research are briefly discussed. The exact diagonalization procedure carried out in thesis is described and also how to obtain current through a mesoscopic interacting system in the Keldysh formalism has been explained. The formula for the current is then used to derive the expression for the conductance through the double quantum dot system at zero and finite temperatures. The single-walled carbon nanotubes used as the leads are also briefly described.

The studies carried out for the double quantum dot system in two geometries incorporates many system parameters mentioned above. In first study, using exact diagonalization the eigenstates of the system are analytically calculated in each particle and spin sectors. Using these results which incorporate all tunable parameters of the system, spin-spin correlation between the dots and the corresponding dot occupancies are calculated as a function of system parameters in the ground state of the half-filled system identified from four dimensional space. The model calculations show that depending on the set of values of ondot Coulomb interaction and interdot tunneling matrix-element, the spins at two dots form either a singlet or triplet. Even in the absence of interdot tunneling matrix-element these correlations are present through indirect exchange via leads. There is a critical dependency of the interdot tunneling matrix-element on the ondot Coulomb interaction which leads to the transition from the ferromagnetic correlation to the antiferromagnetic or vice-versa. The interdot interaction affects this dependency considerably as it renormalizes the ondot interactions. The interdot tunneling matrix-element and ondot Coulomb interaction affect the occupancies of

the dots in such a way that a large value of ondot Coulomb interaction causes the occupancies of the dots to be restricted less than one whereas the interdot tunneling matrix-element causes interdot charge transfer. The interplay of these two effects lead to different spin configurations of the dots.

In T-shaped geometry, at zero temperature it is observed that an antiferromagnetic correlation between the dots is present for finite values of interdot tunneling matrix-element. The antiferromagnetic correlation between the dots changes remarkably for large values of ondot Coulomb interaction both at zero as well as finite temperatures. The spin-spin correlation between the dots is significantly reduced even for small values of the interdot Coulomb interaction compared to the ondot Coulomb interaction. At a small value of temperature, the spin-spin correlation between the dots exhibits a (negative) maximum due to contributions coming from thermal excitations to low-lying states.

The analysis of double quantum dot system is extended and transport properties at zero and finite temperatures of T-shaped system are studied using Keldysh non-equilibrium Green function technique. The linear conductance profile and dot occupancies are calculated. In case of non-interacting electrons, the Fano-antiresonance is observed wherein the linear conductance vanishes (despite occupancies on the dots being finite) whenever the energy level of the quantum dot not directly connected to the leads, aligns with the Fermi energy of the electrons in the leads at zero-bias. This is understood in terms of destructive interference between several possible Feynman paths between the source and drain. The effect of electron-electron correlations on the anti-resonance point present in the non-interacting case, is investigated via ondot and interdot Coulomb interactions within Hartree-Fock as well as beyond Hartree-Fock approximations. Results obtained with beyond Hartree-Fock approximation for Green functions show that the ondot Coulomb interaction on the quantum dot not directly connected to the leads removes the anti-resonance point and leads to splitting of anti-resonance valley into two dips in the linear conductance profile.

Lastly, the temperature dependence study on the transport through T-shaped double quantum dot system when connecting leads are taken as the metallic single-walled carbon nanotube is carried out. Armchair carbon nanotubes with chirality (5,5) and (6,6) have been taken due to their metallic character. As the dot levels can be made to align with a van-Hove singularity present in the density of states of the carbon nanotube leads. The results show that, whether any of the two dot levels align with the van-Hove singularity position in the carbon nanotube leads or not, the heights of the alternate conductance peaks are suppressed and depend on the relative positions of the dot levels and separations between them. But when the one-electron ground state of the isolated double quantum dot system align with the first van-Hove singularity position the height of the corresponding conductance peak falls considerably. This happens due the fact that the eigenstate of the system de-localized over entire Source-Dots-Drain system and the probability amplitude of an electron to occupy the double quantum dot system decreases.