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Referee report on PhD dissertation presented by Mr S.B. Tooski

The dissertation „Quantum entanglement, Kondo effect, and electronic transport in quantum dots system" was written by Mr. Sahib Babaee Tooski in the Institute of Molecular Physics Polish Academy of Sciences in Poznan, Poland. The presented work was performed with the supervisor prof. dr hab. Bogdan Bulka. The thesis is 123 page long, contains 7 chapters, list of publications, conferences presentations and bibliography, 129 items. The thesis is written in English.

In Chapter 1 the author presents aim of his study and outline the general structure of his dissertation. It is focused on two systems: trimers, i.e. triple quantum dots coupled to electrodes, and a quantum dot coupled to electrodes via assisted (correlated) hopping. In Chapter 2 the general introduction to quantum entanglement is presented. As a measure of entanglement the author introduced the concurrence and related it to different correlation functions in spin systems. Later the Kondo effect in presented and the single impurity Anderson model and the Kondo model are discussed. In final sections the conductance and the thermopower are defined and discussed in the context of the Kondo effect. In the last section quantum phase transitions are mentioned. This is useful Chapter, introducing the reader to the main parts of the thesis. Some interpretation of entanglement and EPR scenario are not presented with the sufficient precision but the subject is hard and touches philosophical discussion.

In Chapter 3 the Wilson numerical renormalization group (NRG) is introduced and discussed in some details along a standard way. It is the numerical method used in this thesis to solve problems of quantum dots with correlations and coupled to electric pads. Few thermal static and dynamic observables are presented which are obtained within the NRG procedure. In the course of his investigation Mr. Tooski used a publicly open cod of NRG from Ljubljana group. In my research team we are using the same code with positive experience.

Chapter 4 is the first of three Chapters which present author's results and achievements. In this Chapter he models a system build of three quantum dots coupled to each other by hopping amplitudes and one of the dot is in addition coupled to source and drain electrodes. Electrons on each dot are correlated via the Hubbard local interaction U. Firstly the trimer problem is solved when coupling to electrodes is absent and within the assumption that each dot is single occupied. Such a problem is effectively modeled by the Heisenberg type Hamiltonian and is exactly solvable. The ground states are identified and the quantum phase transitions (level crossings) are found. Different correlators are determined analytically. The role of the electrodes is modeled in the simplest case by the fourth spin which leads to exact solution of that atomic Heisenberg system. When the electric pads are coupled to the trimer the problem is no longer analytically solvable and the author used the NRG method to obtain the physical quantities and the phase diagrams. The main results are shown in the graph 4.2 and 4.3. The concurrence, the spin-spin correlators, charge fluctuations, entropy, local magnetic susceptibility, and conductance are presented in details. The NRG results are nicely interpreted within the effective Heisenberg atomic models and the physics of the system is very transparent and well presented. In particular the S=1/2 and S=1 cases and transition between them are interesting and, perhaps surprisingly, described by discontinuous local phase transition or the phase transition of the local Kosterlitz – Thouless type. Also the monogamy concept is well illustrated on this example.

Chapter 5 continues the study on trimers and shows how to understand the physics away from the single occupancy limit of each dot. Various correlators and occupancies are presented both in the atomic (no electrodes) limit and in the full model. The former is solved analytically and the latter is solved by NRG. The comparison and the agreement in physical understanding of the two limits is remarkable. Two different situations depending on the coupling strength between dots, which are not coupled to electrodes, are identified, i.e. ferromagnetic or antiferromagnetic case. In sec. 5.3 a general derivation of the Friedel sum rule for local Fermi liquid (S=1/2) and local non-Fermi liquid (S=1) is presented. The impurity charge, via the scattering phase shift is related to the conductance. Finally the conductance is determined from the NRG procedure and it is presented in both regular and singular limits.

In Chapter 4 a different topic is presented, namely, the quantum dot coupled to electric pads via correlated hopping type of tunneling. It was shown that the correlated (assisted) hopping changes the conductance and the thermopower because of the renormalization of the dot levels. The change of sign of the thermopower is found to be an important signature of the Kondo-correlated quantum dot. The conclusions are obtained within the NRG method as well as semi-analytical approximations, i.e. Hubbard I.

Chapter 7 provides conclusions and the main achievements of this PhD work.

The dissertation contains many good sides: material is presented with many details, is well written, discussion is well taken, simple atomic limits are used to interpret physical picture and provides physical intuition. The models and systems considered in that thesis are interesting and relevant to current research works ongoing in different laboratories. Many aspects and results touches the most fundamental aspects of quantum mechanics, entanglement, correlations, and how they can affect observables. The obtained results seems to be original and were published in peer review journals.

To the week sides I should count few things: although many times the author refers to experimental possibilities I could not find any estimates of parameters and the results which would correspond to ongoing experimental probes. Arbitrary units are not clearly defined, though experienced reader can get them easily. But it would be desirable to correlated particular results with trimer dots produced in particular labs. Data are available in papers. I also would encourage the author to discuss in details his results in the context of other similar papers from the D. Logan's group, already published. They also studied the similar systems and some results and notions, e.g. Kosterlitz-Thouless transitions in trimers, were predicted. [J. Phys. Chem. B17, 12777 (2013), Phys. Rev. B 79, 085124 (2009), ibid. 81, 075126 (2010)]. To cite those papers along I found not enough. There were some typos or language misprints, which is of minor relevance.

In conclusions, I recommend to let the dissertation for public discussion and I opt for giving a PhD degree to Mr. Tooski. The four published papers and the presented thesis fulfills a formal and custom requirements for that.

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