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Report on the doctoral thesis 'Quantum entanglement, Kondo effect, and electronic transport in quantum dot system' by Sahib Babaee Tooski

Sahib Babaee Tooski has studied undergraduate physics (1999-2004) at the University in Tehran (Iran), where he obtained bachelor title in the solid state physics. Three years later, in 2007, he has completed graduate studies at the Technical University in Tehran (Iran). After the university studies he has received a fellowship from the Iranian Nanotechnology Intuitive Council (2007-2010) for exploring the single-wall carbon nanotubes as potential sensors of the toxins/pollutant gas pressure and other related projects on the functionalized carbon nanotubes.

In 2010 S.B. Tooski has successfully applied for another (3-year) Marie Curie fellowship in the Institute of Molecular Physics of the Polish Academy of Sciences in Poznań (Poland). This position was available within the NanoCTM (Nanoelectronics: Concepts, Theory and Modeling) network funded by the European Commission to create the innovative nano-scale electronic devices. Under supervision of professor Bogdan R. Bułka he has investigated the correlation effects in nanoscopic objects and analyzed their influence on the transport properties. In particular, he has considered a triple quantum dot configuration that is hoped to be stable on decoherence, enabling a realization of the quantum bits (qubits). Within the NanoCTM and the project DEC-2012/05/B/ST3/03208 (financed by the National Science Centre) S.B. Tooski has investigated the following physical issues:

i) quantum entanglement between electron spins in a triple quantum dot coupled to two external electrodes,
ii) quantum phase transition from the screened to underscreened Kondo state driven by a gate voltage and/or inter-dot coupling
iii) the Friedel-Luttinger sum rule and its influence on electron transport properties through a triple quantum dot,
iv) role of the assisted hopping in transport phenomena via the correlated quantum dot.

He has addressed these physical problems using the nonperturbative scheme of the Wilsonian numerical renormalization group (NRG) technique. For specific computations he has adopted a free-available version of the Ljubljana NRG code.

Scientifically guided by prof. Bogdan R. Bułka and in a collaboration with prof. Anton Ramšak and dr. Rok Žitko from J. Stefan Institute in Ljubljana (Slovenia) Sahib B. Tooski has obtained a number of valuable results. His results have been discussed with a scientific community during various international conferences organized in Poland and abroad. He has presented 8 posters (in Hungary, Spain, France, and Poland) and one oral talk during the Capri Spring School on Transport in Nanostructures (Capri, Italy). He has been also invited to give a seminar in the Institute of Physics at M. Curie Skłodowska University (Lublin, Poland). The original results obtained by S.B. Tooski have been already published in: New J. Phys. (1 article), Eur. Phys. J. B (2 articles), Acta Phys. Polon. A (1 article) and another manuscript is the hands of referees. In what follows, I shall point out the major achievements by S.B. Tooski which are summarized in his doctoral thesis.

The present Ph.D. thesis consists of 6 chapters. The first part provides a motivation and a general outline of the theoretical studies conducted by the author for a triple quantum dot. In the second chapter he introduces several useful concepts, related to: 1) concurrence (as a quantitative measure of the quantum entanglement), 2) the Kondo effect (emphasizing its experimental signatures and theoretical interpretation), 3) microscopic Hamiltonian for description of the correlated quantum impurities in terms of the Anderson and/or Kondo scenarios, 4) manifestation of the Kondo effect in electronic transport through the correlated quantum dots (seen in the differential conductance and thermopower), and 5) quantum phase transitions. In a triple quantum dot the quantum phase transition can be triggered between various symmetry ground states of the system by the inter-dot coupling (hybridization) combined with the influence of external leads.

The third chapter gives a general overview the NRG idea for projecting the Anderson impurity problem on the semi-infinite chain, with a logarithmic discretization of the conduction band degrees of freedom. This mapping allows to study the correlations within the iterative renormalization group procedure. By numerical diagonalization of the trigonal Hamiltonian matrix one then obtains the eigen-energies and eigen-vectors. Using these eigen-values/vectors one can determine all the thermodynamic quantities (entropy, internal energy, specific heat) and construct the dynamical correlation functions (making use of the Lehmann representation). The author clearly discussed also technicalities concerning the particular Ljubljana NRG version, comprising: SNEG Mathematica package (for symbolic computations), C++ code (for executing the NRG iteration loop), and two LAPACK libraries (for a diagonalization). S.B. Tooski has installed this NRG-code on 2 computer clasters in the Institute of Molecular Physics PAS in Poznań.

In the fourth chapter the author considers an entanglement of the triple quantum dot (TQD) states originating from two different Kondo effects, depending on the specific couplings. His qualitative and quantitative analysis is done for the configuration where only one quantum dot is laterally coupled with external reservoirs while the other dots are side-attached to it. In section 4.3 the author studies the ground state properties of the isolated TQD. Next, he presents the NRG results obtained for the strongly correlated limit ($U = 10\Gamma$) deep in the Coulomb blockade valley ($\varepsilon = -\frac{U}{2}$) when each quantum dot is occupied nearly by a single electron. The essential findings are displayed in figure 4.2. The physical observables clearly exhibit the quantum phase transition when the interdot couplings $t_1 = t_3$ coincide with the critical value t_{2c} (dependent on Γ). In agreement with the monogamy rule, the maximal concurrence $C_{AB} = 1$ implies the other spins to be non-entangled $C_{AC} = 0 = C_{BC}$. For this reason, upon crossing the critical coupling t_{2c} the concurrence C_{AB} (varying between 0 and 1) simultaneously affects the concurrence C_{AC}. The distinct quantum states are separated by a first order phase transition. On a microscopic level such transition is evidenced by an abrupt change of the spin-spin correlation function $\langle \mathbf{S}_A \cdot \mathbf{S}_B \rangle$ at the critical coupling t_{2c}. Both side-coupled quantum dots evolve between the singlet and triplet states. For $t_2 > t_{2c}$ the vanishing entropy indicates that the side-attached quantum dots form a singlet (with a total spin $S = 0$) and the inter-facial quantum dot is fully screened by itinerant electrons. On the other hand, for weaker coupling t_2 the side-attached dots arrange themselves into $S = 1$ triplet that is underscreened (with characteristic entropy $k_B \ln 2$). The quantum phase transition between such distinct Kondo states is manifested also in the spin susceptibility and the differential conductance. The underscreened Kondo state does completely block any charge transport, whereas the screened Kondo state gives rise to the enhanced zero-bias conductance reaching the perfect (unitary limit) value $2e^2/h$. Finally, the author considers a changeover to the Kosterlitz-Thouless transition when the side-attached dots are no longer symmetrically coupled $t_1 \neq t_3$. Under such circumstances the sharp phase transition is replaced by a smooth one, as can be seen in figure 4.4 in the concurrence as well as the spin-spin correlation function.

In 5-th chapter the author explores the ground state properties of the TQD upon varying a gate voltage, that effectively lifts the energy level ε and affects the electron occupancy. He starts, studying analytically the ground state of the isolated TQD for various relationships between t_1 and t_2 (assuming $t_1 = t_3$). The total electron occupancy shows a step-like variation and reveals the Coulomb-blockade feature (corresponding to $n_{tot} = 3$). Individual spins and the spin-spin correlation functions are very sensitive to the ferromagnetic/antiferromagnetic exchange interactions induced between the quantum dots. This is particularly pronounced in the Coulomb blockade, for the gate voltage region corresponding to $n_{tot} = 3$. S.B. Tooski confronted such results with the NRG calculations obtained at low temperature for the finite (non-vanishing) coupling Γ to external electrodes. External leads are predominantly responsible for a smooth variation of the interfacial (C) quantum dot occupancy with respect to the gate voltage due to its level-broadening. Quantum phase transition between the screened/underscreened Kondo states induces additional qualitative changes in the spin-spin correlations. This can be seen in figures 5.4c (for $t_1 > t_2$) and 5.5c (for $t_1 < t_2$) by abrupt changes at the energy crossings between the screened/underscreened Kondo states.

In section 5.3 the author recalls the useful Friedel-Luttinger sum rule, to express the displacement charge in terms of the T-matrix phase shift. In this context the author emphasizes importance of the Luttinger integral I_L, defined in equation (5.24). Such quantity vanishes for the regular Fermi liquids and it takes $\pi/2$ value for the singular Fermi liquids. This information allows to examine the linear conductance of the TDQ-junction at zero temperature. The zero-bias conductance indeed exhibits a qualitative changeover when the system evolves between two fundamentally distinct ground states. This observation is evident from a comparison of the spectral function (at zero energy) computed directly for the NRG method with the value determined by the Friedel-Luttinger sum rule. In the latter case the local displacement charge is assumed to be identical with the total charge of the triple quantum dot 'molecule'.

The 6-th chapter is devoted to the single quantum dot symmetrically coupled between two external metallic electrodes. Apart of the strong intradot repulsion U Sahib B. Tooski takes into account the assisted (correlated) hopping term, that formally represents off-diagonal matrix element $xV \equiv \langle cf|e^2/r|ff\rangle$ of the Coulomb potential. This term promotes an electron hopping, provided that the quantum dot is occupied by another electron of opposite spin. Such assisted hopping violates the particle-hole symmetry of the quantum dot. Furthermore, it qualitatively affects the electronic spectrum (renormalizing the single particle excitations) and strongly modifies the exchange interaction J_K responsible for the Kondo effect. The latter property is shown by the author analytically from estimations based on the perturbative Schrieffer-Wolf transformation. J_K is found to be a parabolic function of the assisted hopping x. For the half-filled quantum dot its minimum occurs at $x = 1$. The NRG calculations (carried for $U/\Gamma = 8$) confirm that the spin-spin correlation function $\langle \mathbf{S}_f \mathbf{S}\rangle$ reveal indeed the antiferromagnetic spin alignment. Negative value of the correlation function diminishes in magnitude upon increasing x, as displayed in Fig. 6.1d. The local moment (needed for the Kondo effect) is formed only nearby the half-filling. However, for $x \neq 0$, the particle-hole (p-h) symmetry is completely absent. The missing p-h symmetry is observed in the high-energy spectral function (Fig. 6.2a) as well as in the low-energy Abrikosov-Suhl peak (Fig. 6.2b).

Since the assisted (correlated) hopping quenches the upper quasiparticle peak at $\varepsilon + U$, this also substantially affects the transport properties. In section 6.4 the author studies variation of the differential conductance and the thermopower with respect to the gate voltage [and versus total occupancy $\langle n\rangle$] for two representative temperatures, above and below T_K. At high temperature ($T > T_K$) the zero-bias conductance reveals the Coulomb blockade peaks, with the lower one strongly dependent on x (because the quasiparticle peak is narrowed). As far as the thermopower is concerned it roughly obeys the Mott relation, being proportional to a derivative of the conductance. These NRG results can be well reproduced by the Hubbard-I approximation (capturing the Coulomb blockade features). In the Kondo regime the asymmetric Abrikosov-Suhl peak has a pronounced effect both, on the Seebeck coefficient and on the conductance. With increasing x the zero-bias conductance essentially deviates from the unitary limit value due to the suppressed Kondo temperature that controls a width of the Abrikosov-Suhl peak. The gate-dependent conductance tends then to a single broad maximum, whereas the thermopower exhibits a single sign change. Overall temperature variations of the thermopower and the conductance are summarized by the author in figure 6.7.

The present doctoral thesis is very clearly written and well organized. Each chapter provides the useful information about the discussed physical issue and is carefully summarized along with an outlook. I have just a few critical remarks regarding the editorial side. In sections 5.1 and 5.2 the author mentions the statistical expectation values $\langle n_{tot}\rangle$ and $\langle S_i^2\rangle$ referring to them as '*correlators*'. In my opinion, the correlators (or correlation functions) are reserved for the products $\langle O_i O_j\rangle$ of two (or more) different observables $O_i \neq O_j$, for instance $\langle \mathbf{S}_A \mathbf{S}_B\rangle$. Next, in section 5.2, the author discusses the NRG results for the model Hamiltonian (5.1), however, he does not specify a value of the inter-dot Coulomb potential U_1. Presumably, this potential was either neglected or assumed to be much smaller than the intra-dot repulsion $U/\Gamma = 20$. I noticed some typos while reading the main text. For instance, the author often repeats the phrase '*lets me consider ...*' instead of the correct '*let me consider ...*' or '*lets consider ...*'. Such and other similar typos are rather meaningless, therefore I don't change my very positive opinion about the present thesis.

In summary, Sahib B. Tooski has obtained a number of valuable and nontrivial results. He has gained a deep knowledge about the NRG technique and its practical computer implementation. He has proved to be good expert of the Kondo physics both, for the single Anderson impurity and for multiple quantum dot structures. He is familiar with various many-body techniques and has a broad knowledge about the transport phenomena through nanoscopic objects. I am convinced that **Sahib Babaee Tooski fully deserves to obtain the Ph.D title** in physics. Moreover, I think that his considerations of the assisted hopping are very original and they may stimulate completely new studies of the correlations (like the spin and/or charge Kondo effects) driven by the off-diagonal matrix elements of the Coulomb potential. For this reason, I recommend **the present doctoral thesis to be distinguished**.

Tadeusz Domański
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