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WPŁYNĘŁO

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Referee's report on the PhD thesis of **Banhi Chatterjee** entitled
Screening and Friedel oscillations in inhomogeneous systems with correlated fermions

The reviewed PhD thesis has been prepared under supervision of prof. Krzysztof Byczuk from Institute of Theoretical Physics of Warsaw University and dr Krzysztof Makuch from Institute of Physical Chemistry of Polish Academy of Sciences. The work deals with theoretical studies of Friedel oscillations in strongly correlated inhomogeneous fermion systems. They appear in metals at low temperature in the neighbourhood of a charged impurity. The Hubbard model has been used to description of these systems and has been solved numerically by means of the Real Space Dynamical Mean-Field Theory (R-DMFT) with the use of various approximations. Oscillations have been investigated for metals, insulators and the Mott insulating phase. Moreover, the effect of correlations and temperature on the screening charge and spectral functions at different lattice sites in one- two- and three-dimensional systems was studied. Some results of the thesis were published in *Journal of Physics* 592 (2015) 012059 and were presented at many conferences and at international workshops.

The PhD thesis is well structured and contains 150 pages divided into nine main chapters. At the beginning lists of figures, symbols and abbreviations are introduced. Finally, summary, outlook and open questions, three appendices, bibliography and authors scientific contribution and training are presented. Reviewed work includes 105 figures and 132 references.

The first chapter introduces topics and explains the motivations behind applied numerical technics for solving problems.

The second chapter gives an overview of the historical background of Friedel oscillations both in the theory and experiment. It shows that the current stage of quantitative analysis of these oscillations is not sufficient enough if screening effects caused by the impurities in correlated systems occur around the Mott transition. Hence, it was a strong incentive of the Author to take up studies concerning this matter.

The third chapter exhibits the properties and classification of strongly correlated systems. It was shown that fermionic optical lattices are adequate to study the Mott transition.

The next chapter is an elementary introduction to the Hubbard model with inhomogeneous potentials which is the simplest model to depict strongly correlated systems. Unfortunately, the exact solutions of this model exist only in one-dimensional lattices. In view of the fundamental limitations of exact analytical approaches it is indispensable to choose the approximate methods in higher dimensions. However, since the number of quantum mechanical states increases exponentially with the number of lattice sites, numerically exact solutions are limited to small systems (a dozen of lattice sites). Furthermore, solutions of the inhomogeneous Hubbard model and arguments to choose approximate methods are clearly shown.

The fifth chapter contains the Green's function approach, equations of motion for inhomogeneous Hubbard model and a detailed derivation of equations of the Dynamical Mean-Field Theory (DMFT) using cavity method. It has been shown that the effective local action of DFMT is equivalent to single impurity Anderson model. Next the algorithm to solve the self-consistent DFMT and collection of various methods both numerical and analytical was very neatly presented. The extension called R-DFMT (a real space extension) useful for solving inhomogeneous systems was also shown. In the framework of R-DFMT the generalized Friedel sum rule (FSR) for interacting systems was derived in T-matrix approach. In the last part of this chapter the analytical formula for Friedel oscillations in the presence of a localized impurity potential was derived. I recommend this chapter to the beginners in DFMT formalism as a good introduction.

The sixth chapter is the central point where the screening and Friedel oscillations in correlated inhomogeneous systems were comprehensively studied. The following physical quantities were numerically calculated in the presence of single site impurity potential: i) local spectral functions; ii) local occupation of electron per lattice site and the electronic density; iii) N-site charge. These quantities were obtained by solving the Hubbard model applying numerical exact R-DFMT + CTQMC method (continuous time quantum Monte Carlo) for finite systems with periodic boundary conditions. All the inhomogeneities in the self-energy were also taken into account. The method works effectively for finite temperature only and it is worse for zero temperature (it is a time-consuming numerical method). Hence, other approximate methods to study oscillations in the limit of low temperature were applied: approximation A (a self-energy model) in metallic phase and approximation B in insulating phase (the self-energy under Hubbard I approximation). Approximation C (Numerical Renormalization Group NRG) and exact numerical method (R-DFMT+CTQMC) presents uniquely a complete picture both for metallic and insulating regime. Numerical calculations clearly show that the effects of interaction and temperature on Friedel oscillations both for finite and zero temperature are similar. Results obtained in this approach testify physical credibility of the applying methods.

The seventh and eighth chapters are the research extensions of the sixth chapter to the finite systems with two\ multiple single-site impurities and extended inhomogeneity for one and two dimensional systems.

In the ninth chapter semi-analytical calculations using the model Bethe density of state and the self-energy model for a single impurity is presented as well as an analytical approach

to explain the behaviour of the spectral function using Hubbard I self-energy in the presence of single impurity.

The last chapter indicates the direct extension of this thesis and points out the new routes for both theoretical and experimental studies of Friedel oscillations in correlated systems.

The three appendices closing the disertation contain:

- i) appendix A: the estimation of critical interaction and temperature for Mott transition in finite systems;
- ii) appendix B: mapping the Hamiltonian of higher dimensional lattices into equivalent one-dimensional systems and
- iii) appendix C: technical numerical details of R-DFMT+CTQMC calculations.

The thesis refereed by me represents a meticulous analysis. The emphasis is put on the computationally reliable description rather than on basic analytical calculations.

I want to stress that the following new findings for the unhomogeneous correlated finite systems with periodic boundary conditions were obtained for the first time:

- for all dimensions d Friedel oscillations decay with the relative distance from the impurity as $1/r^d$ both for interacting and non-interacting systems;
- at half-filling the amplitude of Friedel oscillations decreases with the interactions and temperature while the period and phase of this oscillations remains unchanged;
- excellent result of disappearing Friedel oscillations at the Mott transition and no oscillations beyond it in the insulating phase;
- the replacement of a bound state by a resonance at the impurity site when the interactions are switched on;
- the universality in the variation of the N-screening charge with the impurities and interactions for the one, two and three dimensional case;
- the Friedel sum rule works correctly when inhomogeneities in the self-energy is taken into account;
- interactions weaken the interference effects between the impurities;
- the system becomes more homogeneous with increasing interactions for spin independent models in the presence of extended inhomogeneities .

I would suggest studying the Friedel-crystal phases where oscillations in the Coulomb force can be the dominant effect determining the elastic properties in nanocrystal structures. It will be also interesting to explore the influence of magnetic fields on Friedel oscillations controlling.

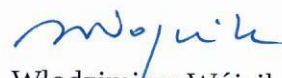
This thesis is perfectly written and has a clear layout. The figures are shown properly as well. The limitations of numerical calculations are under appropriate discussions and possibilities are delineated for future works. The literature review is comprehensive. The work presented shows that the Author has mastered a variety of numerical techniques for studying many-body problems including continuous time quantum Monte-Carlo method.

I believe that the personal effort of Banhi Chatterjee deserves the highest mark.

Nevertheless, I have some remarks. There is a number of typos, e.g. in Eqs (4.3), (4.14), etc., or the Author refers to a nonexistent equation on page 36. Also there is a number of incorrect citations as well as the cited articles are not properly ordered. I also found some inconsistency in pictures, e.g. in Fig. 6.1 each panel is plotted within different convention, or in some plots axis labels and units are not presented accordingly. I think that these are minor points but in the future the Author should be more careful in preparing scientific texts.

In conclusion, my view of the thesis is that it is substantial and well-presented. I have learned some interesting new things from it. The submitted thesis contains high-quality original findings of large importance for correlated finite systems which can be stimulus for the future experiments in nanoscience. One might hope that modern supercomputers can provide detailed numerical insights into the thermodynamic and spectral properties of fermionic models. I also believe that many new unpublished results will be released in the period ahead.

In summary, I am fully convinced that the thesis of Banhi Chatterjee has fulfilled the thesis requirements for a PhD, and I am pleased to recommend it for defense presentation.



Włodzimierz Wójcik