PhD thesis

Theoretical study of gapless low-dimensional systems: graphene and the Luttinger model

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1. Introduction

Low-dimensional systems, i.e. systems with spatial dimensions less than three, have attracted lots of interest lately. Many of these materials are already present in tools of our everyday life (for example in semiconductor based microelectronic circuits), while others are still subject of intense investigations.

One of the most exciting low-dimensional system is graphene which is a quasi two-dimensional material consisting of carbon atoms arranged in a honeycomb lattice. Electrons in graphene are modeled as Dirac fermions described by linear isotropic dispersion relation instead of a parabolic spectrum which is characteristic for free electron gases. Peculiar electronic properties of graphene play an important role in future industrial applications. Therefore, from the theoretical point of view, the most important task is to understand and make predictions on electronic and transport phenomena.

Interaction between electrons and impurities strongly influence transport properties of graphene. This interaction is directly manifestated in the Friedel oscillation which is a short-wavelength oscillation of the electron density with an amplitude decaying as r^{-2} in a two-dimensional free electron gas. In graphene, r^{-2} and r^{-3} both have been predicted but the exponent of the decay has not been measured experimentally yet.

For potential industrial applications, researchers make effort to open a band gap in the bandstructure of grap-

hene. One possible solution could be the artificial tuning of the strength of the interaction between electrons, e.g., via mechanical strain. Due to the weak intrinsic screening of electrons in graphene, Coulomb interaction is expected to play an important role in electronic properties. Therefore, it is an important issue how the interaction affects the bandstructure and under what circumstances is it possible to open a gap. The Hubbard model provides a simple description of the interacting electron system. Former numerical calculation predicted a Mott transition at finite interaction strength and the bandgap was found to vanish linearly near the critical point but no systematic study of the complete critical behavior was performed.

Another interesting property of graphene is the universal behavior of the optical conductivity which is a constant over a wide range of frequency and, moreover, is $\pi/2$ times the conductance quantum. The frequency independent behavior can be explained by the low-energy excitations in graphene. However, it was an open question, which property of the electrons determines fundamentally this universal frequency dependence in graphene and which systems show similar behavior.

Besides graphene, cold atomic systems have also become the subject of intense investigation in the last decade. The parameters of these systems can be tuned very precisely in experiments which allows us to simulate well-known theoretical models, e.g., Bose-Hubbard model and Luttinger model. Time resolved measurements became also available, i.e. the time dependence of various physical qu-

antities can be measured directly. From the theoretical point of view, one of the most important questions is how quantum systems can be described far from equilibrium. In one dimension, many interacting systems can be modeled by the exactly solvable Luttinger model. It is an interesting issue what happens to the model when the system is driven far from equilibrium, e.g., by tuning its parameters non-adiabatically, and how the steady state after relaxation can be described. Integrable models, like the Luttinger model, show no thermalization but the steady state can be described by the so-called diagonal ensemble.

2. Objectives

One main line of my doctoral research is the theoretical investigation of the electronic properties of graphene using analytical methods. The aim is to explore the relation between interesting physical phenomena and the peculiar electronic properties of graphene.

In order to resolve former controversal results on Friedel oscillations, I investigated electron scattering off a well-localized impurity. My goal was to describe the modulation of the local density of states and electron density on the scale of a lattice constant so that I could make predictions on scanning tunneling microscopy measurements with finite spatial resolution.

Coloumb interaction between Dirac fermions is another exciting field of graphene physics. My goal was to study

the critical behavior of a Mott transition within mean-field theory. The unusual critical exponent was the motivation of the extension of the model to general gapless systems with arbitrary power-law energy dependence of the density of states.

In order to understand the universal frequency dependence of monolayer and chirally stacked multilayer graphene, I studied optical transitions of general two-band models. My goal was to determine the class of systems which show universal behavior similar to that of graphene.

Another main line of my doctoral research was the nonequilibrium dynamics of quantum systems. Dynamical properties of the Luttinger model describing one-dimensional interacting systems were investigated mostly with zero initial temperature. My goal was to study finite temperature effects in the diagonal ensemble, which provides a full description of the steady state after a quantum quench. In addition, the objective of my research was to make predictions on the temperature dependence of directly measurable physical quantities, for example the total energy in the steady state or the work done on the system during the quench.

3. New scientific results

The results of my doctoral research are summarized in the following theses.

1. I investigated the atomic scale spatial variations of

the Friedel oscillation in monolayer graphene. In the presence of a well localized impurity, I obtained the change in the local density of states and in the electron density within Born approximation. Far from the impurity, the latter shows long wavelength oscillating behavior with an envelope decaying as r^{-2}. By taking into account the atomic orbitals and intervalley scattering, I showed that the leading correction vanishes in an STM experiment with spatial resolution worse than three unit cells. In the absence of intervalley scattering, a resolution worse than one unit cell already leads to cancellation leaving us the next-to-leading r^{-3} correction. The results are published in Ref. [1].

2. I studied the critical behavior of an antiferromagnetic quantum phase transition in undoped monolayer graphene within mean-field approximation. The critical exponents differ from that of the conventional Landau theory. The resulting unconventional critical behaviour was explained by generalizing the model to systems with arbitrary power law density of states. I derived how the critical exponents of a quantum phase transition depend on the density of states exponent, r, within mean-field theory. As a result, I found significant r-dependence in the $-1 < r < 2$ regime with singular behavior in the limit of constant density of states ($r = 0$). In the $r \geq 2$ region, the critical exponents do not depend on the density of

states exponent and coincide with their conventional value in Landau theory. The results are published in Ref. [2].

3. Using the Kubo formula, I derived analytical expressions for the optical conductivity of generic two-band systems whose quasi-particles possess a pseudospin degree of freedom. I showed that if the pseudospin is determined only by the direction of the particle's momentum, i.e. the particles are chiral in a general sense, the optical condutivity exhibits universal power law frequency dependence with the exponent $(d-2)/z$ where d is the number of spatial dimensions of the system and z is the dynamical exponent. The results are published in Ref. [3].

4. In the Luttinger model, I studied the diagonal ensemble which provides a full description of the steady state after a quantum quench and also coincides with the joint distribution of boson numbers in the momentum channels of the final state. The distribution was analytically obtained for arbitrary quench protocol, interaction strength and for arbitrary initial temperature. For a given channel, the result shows universal behavior in the sense that all information about the quench protocol is incorporated into the expectation value of the boson number. All higher moments are already determined by the expectation value. I showed that for higher initial temperatu-

res, the boson numbers in the q and $-q$ channels are less correlated but are never uncorrelated unless the quench is adiabatic. I found that for higher initial temperatures more bosons are produced during the quench. The results are published in Ref. [4].

5. I investigated the finite temperature effects in the statistics of total energy and work done in the Luttinger model after a sudden interaction quench. After deriving the generating function of the distributions analytically within perturbation theory, the probability distribution functions were evaluated by numerical Fourier transformation. The shape of the distribution depends remarkably on the system size. For small systems, the distributions are significantly deformed as the initial temperature increases. For large system, the total energy distribution is shifted to positive direction, while the expectation value of the work done on the system remains at zero and no significant deformation was found. I showed that the variance of the distributions behaves as $\sim T^3$ at low temperatures. The results are published in Ref. [4].

4. Publications related to the thesis statements

[1] Á. Bácsi and A. Virosztek, Local density of states and friedel oscillations in graphene, *Phys. Rev. B*

82, 193405 (2010)

[2] Á. Bácsi, A. Virosztek, L. Borda and B. Dóra, Mean-field quantum phase transition in graphene and in general gapless systems, *Phys. Rev. B* **82**, 153406 (2010)

[3] Á. Bácsi and A. Virosztek, Low-frequency optical conductivity in graphene and in other scale-invariant two-band systems, *Phys. Rev. B* **87**, 125425 (2013)

[4] Á. Bácsi and B. Dóra, Quantum quench in the Luttinger model with finite temperature initial state, *Phys. Rev. B* **88**, 155115 (2013)

5. Other publications

[5] A. Virosztek and Á. Bácsi, Friedel oscillations around a short range scatterer: the case of graphene, *J. Supercond. Nov. Magn.* **25**, 691 (2012)

[6] B. Dóra, Á. Bácsi, and G. Zaránd, Generalized Gibbs ensemble and work statistics of a quenched Luttinger liquid, *Phys. Rev. B* **86**, 161109 (2012)