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Tobias Brandes (Ed.)

Low-Dimensional Systems

Interactions and Transport Properties

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Interactions and Transport Properties

Lectures of a Workshop Held in Hamburg, Germany, July 27-28, 1999

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Preface

Experimental progress over the past few years has made it possible to test a number of fundamental physical concepts related to the motion of electrons in low dimensions. The production and experimental control of novel structures with typical sizes in the sub-micrometer regime has now become possible. In particular, semiconductors are widely used in order to confine the motion of electrons in two-dimensional heterostructures. The quantum Hall effect was one of the first highlights of the new physics that is revealed by this confinement. In a further step of the technological development in semiconductor-heterostructures, other artificial devices such as quasi one-dimensional 'quantum wires' and 'quantum dots' (artificial atoms) have also been produced. These structures again differ very markedly from three- and two-dimensional systems, especially in relation to the transport of electrons and the interaction with light. Although the technological advances and the experimental skills connected with these new structures are progressing extremely fast, our theoretical understanding of the physical effects (such as the quantum Hall effect) is still at a very rudimentary level.

In low-dimensional structures, the interaction of electrons with one another and with other degrees of freedoms such as lattice vibrations or light gives rise to new phenomena that are very different from those familiar in the bulk material. The theoretical formulation of the electronic transport properties of small devices may be considered well-established, provided interaction processes are neglected. On the other hand, the influence of interactions on quantities such as the conductance and conductivity remains one of the most controversial issues of recent years. Progress has been achieved partly in the understanding of new quasiparticles such as skyrmions, composite fermions, and new states of the interacting electron gas (e.g., Tomonaga–Luttinger liquids), both theoretically and in experiments. At the same time, it has now become clear that for fast processes in small structures not only the interaction but also the non-equilibrium aspect of quantum transport is of fundamental importance. It is also apparent now that, in order to understand a major part of the experimental results, transport theories are required that comprise both the non-equilibrium and the interaction aspect, formulated in the framework of a physical language that was born almost exactly one century ago: quantum mechanics.

This volume contains the proceedings of the 219th WEH workshop 'Interactions and transport properties of low dimensional systems' that took place on July 27 and 28, 1999, at the Warburg–Haus in Hamburg, Germany. Talks were

given by leading experts who presented and discussed recent advances for the benefit of participants from all over the world, among whom were many young students. This is one reason why the present volume is more than simply a state-of-the-art collection of review articles on electronic properties of interacting lower dimensional systems. We have also tried to achieve a style of presentation that allows an advanced student or newcomer to use this as a textbook. Further study is facilitated by the many references at the end of each article. Thus we encourage all those interested to use this book together with pencil and sometimes the further reading, to gain an entry into this fascinating field of modern physics.

The articles in Part I present the physics of interacting electrons in one-dimensional systems. Here, one of the key issues is the identification of power-laws appearing as a function of energy scales such as the voltage, the frequency, or the temperature. A generic theoretical description of the physics of such systems is provided by the Tomonaga–Luttinger model, where in general power-law exponents depend on the strength of the electron–electron interaction. Further important issues are the proper definition of the conductance of interacting systems, the experimental verification of the predictions, and the search for new phases in quantum wires, as discussed in detail in the individual contributions.

The articles in Part II present an introduction to non-equilibrium transport through quantum dots, a survey of spin-related effects appearing in electronic transport properties, and new phenomena in two-dimensional systems under quantum Hall conditions, i.e. in strong magnetic fields.

All the contributions contain new and surprising results. One can definitely predict that many more novel aspects of the physics of 'interactions plus non-equilibrium in low dimensions' will emerge in the future. At this point, let me express the wish that this book will help to motivate readers to take part in this fascinating, rapidly developing field of physics. I would like also to use the present opportunity to thank all the participants and the speakers of the workshop for their contributions, and to acknowledge the friendly support of the WE Heraeus foundation.

Hamburg, November 1999 *Tobias Brandes*

Contents

Part I

Transport and Interactions in One Dimension

Nonequilibrium Mesoscopic Conductors Driven by Reservoirs

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Abstract. In order to specify a nonequilibrium steady state of a quantum wire (QWR), one must connect reservoirs to it. Since reservoirs should be large 2d or 3d systems, the total system is a large and inhomogeneous 2d or 3d system, in which *e-e* interactions have the same strength in all regions. However, most theories of interacting electrons in QWR considered simplified 1d models, in which reservoirs are absent or replaced with noninteracting 1d leads. We first discuss fundamental problems of such theories in view of nonequilibrium statistical mechanics. We then present formulations which are free from such difficulties, and discuss what is going on in mesoscopic systems in nonequilibrium steady state. In particular, we point out important roles of energy corrections and non-mechanical forces, which are induced by a finite current.

1 Introduction

According to nonequilibrium thermodynamics, one can specify nonequilibrium states of macroscopic systems by specifying local values of thermodynamical quantities, such as the local density and the local temperature, because of the local equilibrium [1,2]. When one studies transport properties of a mesoscopic conductor (quantum wire (QWR)), however, the local equilibrium is not realized in it, because it is too small. Hence, in order to specify its nonequilibrium state uniquely, one must connect *reservoirs* to it, and specify their chemical potentials ($\mu_{\rm L}$, $\mu_{\rm R}$) instead of specifying the local quantities of the conductor (Fig. 1). The reservoirs should be large (macroscopic) 2d or 3d systems. Therefore, to really understand transport properties, we must analyze such a composite system of the QWR and the 2d or 3d reservoirs, Although the QWR itself may be a homogeneous 1d system, the total system is a *2d or 3d inhomogeneous system* without the translational symmetry. Moreover, *many-body interactions* are important *both* in the conductor and in the reservoirs: If electrons were free in a reservoir, electrons could neither be injected (absorbed) into (from) the conductor, nor could they relax to achieve the local equilibrium. However, most theories considered simplified 1d models, in which reservoirs are absent or replaced with noninteracting 1d leads [3–12].

In this paper, we study transport properties of a composite system of a QWR plus reservoirs, where *e-e* interactions are present in all regions. By critically reviewing theories of the conductance, we first point out fundamental problems of the theories in view of nonequilibrium statistical mechanics. We then present formulations which are free from such difficulties, and discuss what is going on in mesoscopic systems in nonequilibrium steady state. In particular, we point

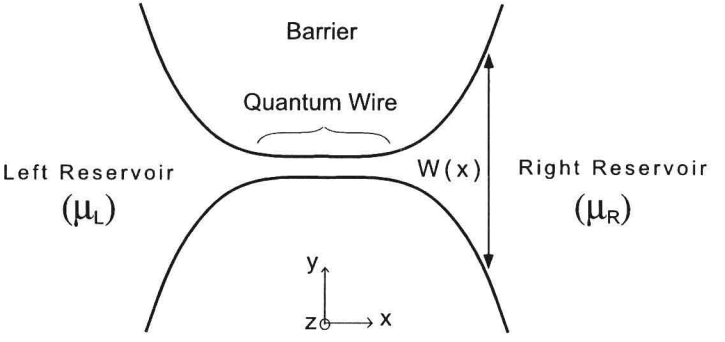


Fig. 1. A two-terminal conductor composed of a QWR and reservoirs.

out important roles of energy corrections and non-mechanical forces, which are induced by a finite current.

2 A Critical Review of Theories of the DC Conductance

In this section, we critically review theories of the DC conductance G of interacting electrons in a QWR. Note that two theories which predict different nonequilibrium states can (be adjusted to) give the same value of G (to agree with experiment). Hence, the comparison of the values of G among different theories is not sufficient. For definiteness, we consider a two-terminal conductor composed of a quantum wire (QWR) and two reservoirs (Fig. 1), which are defined by a confining potential u^c, at zero temperature. Throughout this paper, *we assume that u^c is smooth and slowly-varying, so that electrons are not reflected by u^c* (i.e., the wavefunction evolves adiabatically). We also assume that only the lowest subband of the QWR is occupied by electrons. A finite current I is induced by applying a finite difference $\Delta\mu = \mu_L - \mu_R$ of chemical potentials between the two reservoirs, and the DC conductance is defined by $G \equiv \langle I \rangle / (\Delta\mu/e)$ [13], where $\langle I \rangle$ is the average value of I.

Let us consider a clean QWR, which has no impurities or defects. For *non-interacting* electrons the Landauer-Büttiker formula gives $G = e^2/\pi\hbar$ [14], whereas G for *interacting* electrons has been a subject of controversy [15]. Most theories before 1995 [3–6] predicted that G should be "renormalized" by the e-e interactions as $G = K_\rho e^2/\pi\hbar$, where K_ρ is a parameter characterizing the Tomonaga-Luttinger liquid (TLL) [16–19]. However, Tarucha et al. found experimentally that $G \simeq e^2/\pi\hbar$ for a QWR of $K_\rho \simeq 0.7$ [20]. Then, several theoretical papers have been published to explain the absence of the renormalization of G [8–12,21]. Although they concluded the same result, $G = e^2/\pi\hbar$, the theoretical frameworks and the physics are very different from each other. Since most theories are based either on the Kubo formula [22] (or, similar ones based on the adiabatic switching of an "external" field), or on the scattering theory, we review these two types of theories critically in this section.

2.1 Problems and Limitations of the Kubo Formula when Applied to Mesoscopic Conductors

When one considers a physical system, it always interacts with other systems, R_1, R_2, $\cdots$, which are called heat baths or reservoirs. Nonequilibrium properties of the system can be calculated if one knows the reduced density matrix $\hat{\zeta} \equiv \mathrm{Tr}_{R1+R2+\cdots}[\hat{\zeta}_{\mathrm{total}}]$. Here, $\hat{\zeta}_{\mathrm{total}}$ is the density operator of the total system, and $\mathrm{Tr}_{R1+R2+\cdots}$ denotes the trace operation over reservoirs' degrees of freedom. To find $\hat{\zeta}$, Kubo [22] assumed that the system is initially in its equilibrium state. Then an "external field" $\mathbf{E}_{\mathrm{ext}}$ is applied adiabatically (i.e., $\mathbf{E}_{\mathrm{ext}} \propto e^{-\epsilon|t|}$), *which is a fictitious field* because it does not always have its physical correspondence (see below). The time evolution of $\hat{\zeta}$ was calculated using the von Neumann equation of an isolated system; i.e., *it was assumed that the system were isolated from the reservoirs* during the time evolution [2]. Because of these two assumptions (the fictitious field and isolated system), some conditions are required to get correct results by the Kubo formula. To examine the conditions, we must distinguish between *non-dissipative responses* (such as the DC magnetic susceptibility) and *dissipative responses* (such as the DC conductivity σ). The non-dissipative responses are essentially equilibrium properties of the system; in fact, they can be calculated from *equilibrium* statistical mechanics.

For non-dissipative responses, Kubo [22,23] and Suzuki [24] established the conditions for the validity of the Kubo formula, by comparing the formula with the results of equilibrium statistical mechanics: (i) The proper order should be taken in the limiting procedures of $\omega, q \to 0$ and $V \to \infty$, where ω and q are the frequency and wavenumber of the external field, and V denotes the system volume. (ii) The dynamics of the system should have the following property;

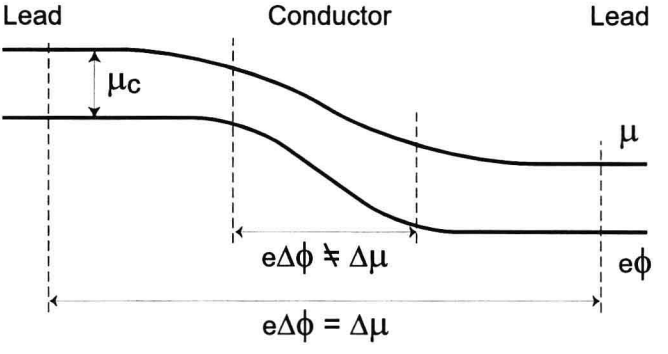
$$\lim_{t\to\infty} \langle \hat{A}\hat{B}(t) \rangle_{\mathrm{eq}} = \langle \hat{A} \rangle_{\mathrm{eq}} \langle \hat{B} \rangle_{\mathrm{eq}}, \tag{1}$$

where $\langle \cdots \rangle_{\mathrm{eq}}$ denotes the expectation value in the thermal equilibrium, and $\hat{A}$ and $\hat{B}$ are the operators whose correlation is evaluated in the Kubo formula. Any integrable models do not have this property [24,26–28]. Hence, *the Kubo formula is not applicable to integrable models, such as the Luttinger model*, even for (the simple case of) non-dissipative responses [24].

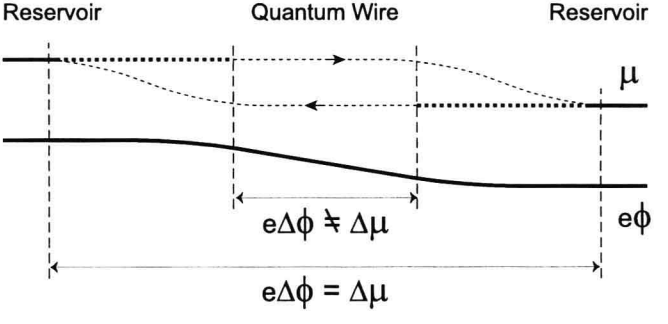
For dissipative responses, the conditions for the applicability of the Kubo formula would be stronger. Unfortunately, however, they are not completely clarified, and we here list some of known or suggested conditions for σ:
(i′) Like as condition (i), the proper order should be taken in the limiting procedures. For σ the order should be [25]

$$\sigma = \lim_{\omega\to 0} \lim_{q\to 0} \lim_{V\to\infty} \sigma_{\mathrm{formula}}(q, \omega; V). \tag{2}$$

(ii′) Concerning condition (ii), a stronger condition seems necessary for dissipative responses: The closed system that is taken in the calculation of the Kubo formula should have the thermodynamical stability, i.e., it approaches the thermal equilibrium when it is initially subject to a macroscopic perturbation. (Otherwise, it would be unlikely for the system to approach the correct steady state



(a) macroscopic inhomegeneous conductor



(b) mesoscopic conductor

Fig. 2. Schematic plots of the chemical potential μ [30] and the electrostatic potential ϕ, for (a) a macroscopic inhomogeneous conductor and (b) a mesoscopic conductor. For case (a), the local equilibrium is established, and thus μ and ϕ can be defined in all regions. The differences $e\Delta\phi$ and $\Delta\mu$ are not equal if one takes the differences between both ends of the conductor, whereas $e\Delta\phi = \Delta\mu$ if the differences are taken between the leads. For case (b), μ cannot be defined in the QWR and boundary regions (although in some cases μ could be defined separately for left- and right-going electrons), whereas ϕ can be defined in all regions. Similarly to case (a), $e\Delta\phi \neq \Delta\mu$ if one takes the differences between both ends of the QWR, whereas $e\Delta\phi = \Delta\mu$ if the differences are taken between the reservoirs.

in the presence of an external field.) In classical Hamiltonian systems, this condition is almost equivalent to the "mixing property" [26–28], which states that Eq. (1) should hold for *any* $\hat{A}$ and $\hat{B}$, where $\langle \cdots \rangle_{\rm eq}$ is now taken as the average over the equi-energy surface. It is this condition, rather than the "ergodicity", that guarantees the thermodynamical stability [26–28]. Although real physical systems should always have this property, some theoretical models do not. In particular, any integrable models do not have this property [26–28].

(iii′) We here suggest that all driving forces, including non-mechanical ones, should be identified [29]. In fact, the formula gives the current density in the following form,

$$\langle \mathbf{J} \rangle = \sigma_{\text{formula}} \mathbf{E}_{\text{ext}}, \tag{3}$$

whereas the *exact* definition of σ is given by nonequilibrium thermodynamics as [1,2]

$$\langle \mathbf{J} \rangle = -\sigma \nabla(\mu/e) - L_{12} \nabla\beta = \sigma \mathbf{E} - \sigma \nabla(\mu_{\text{c}}/e) - L_{12} \nabla\beta. \tag{4}$$

Here, β denotes the inverse temperature, μ is the "chemical potential" which consists of a chemical portion μ_{c} and the electrostatic potential ϕ [1,30];

$$\mu = \mu_{\text{c}} + e\phi \quad \text{(hence, } \Delta\mu = \Delta\mu_{\text{c}} + e\Delta\phi \text{ for differences)}. \tag{5}$$

Hence, to evaluate σ, one must find the relation between $\mathbf{E}_{\text{ext}}$ and $\mathbf{E}$, $\nabla\mu_{\text{c}}$ and $\nabla\beta$. In *homogeneous* systems, it is expected that $\nabla\mu_{\text{c}} = \nabla\beta = 0$, hence it is sufficient to find the relation between the fictitious field $\mathbf{E}_{\text{ext}}$ and the real field $\mathbf{E}$ [2,10,31]. In *inhomogeneous* systems, however, $\nabla\mu_{\text{c}} \neq 0$ and/or $\nabla\beta \neq 0$ in general [32], as shown in Fig. 2 (a). Therefore, one must find the relation between $\mathbf{E}_{\text{ext}}$ and these "non-mechanical forces" [29,33]. (See section 5.)

Unfortunately, these conditions are not satisfied in theories based on simplified models of mesoscopic systems. For example, the Luttinger model [17] used in much literature does not satisfy conditions (i) and (ii) because it is integrable. To get reasonable results, subtle procedures, which have not been justified yet, were taken in actual calculations. Moreover, the non-mechanical forces have not been examined, although they would be important because a mesoscopic conductor (a QWR plus reservoirs) is an inhomogeneous system.

We also mention limitation of the Kubo formula: it cannot be applied to the nonequilibrium noise (NEN), which is the current fluctuation in the presence of a finite current $\langle I \rangle$ $(= G\Delta\mu)$ [7,34–38]. The NEN at low frequency, $\langle \delta I^2 \rangle^{\omega \simeq 0}$, is usually proportional to $|\langle I \rangle| \propto |\Delta\mu|$. However, the Kubo formula assumes power series expansion about $\Delta\mu = 0$, hence cannot give any function of $|\Delta\mu|$ [29,39].

In sections 3 and 4, we present other formulations which are free from these problems and limitations. These formulations clarify what is going on in nonequilibrium mesoscopic conductors, because one can find the nonequilibrium steady state. This is impossible by the Kubo formula because it evaluates correlation functions in the *equilibrium* state.

2.2 Scattering-Theoretical Approaches

In view of many problems and limitations of the Kubo formula, it is natural to try to generalize Landauer's theory [14] to treat conductors with many-body interactions. Namely, the DC conductance may be given in terms of the scattering matrix (S matrix) for interacting electrons [7,11,34].

The advantages of the scattering-theoretical approaches may be as follows: (i) Neither the translation of $\Delta\phi_{\rm ext}$ into $\Delta\mu$ nor the subtle limiting procedures of ω, q and V is necessary. (ii) There is no need for the mixing property of the 1d Hamiltonian $\hat{H}_1$. Hence, $\hat{H}_1$ can be the Hamiltonian of integrable 1d systems such as the TLL. (iii) In contrast to the Kubo formula, one can calculate the NEN [7,34–36].

However, to define the S matrix, one must define incoming and outgoing states. Although they can be defined trivially for free electrons, it is nontrivial in the presence of many-body interactions. In high-energy physics, they are defined based on the *asymptotic condition*, which assumes that particles behave like free (but renormalized) ones as $t \to \pm\infty$, i.e., before and after the collision [40]. For example, an electron (in the vacuum) before or after the collision becomes a localized "cloud" of electrons and positrons, which extend only over the Compton length, and this cloud can be regarded as a renormalized electron. In condensed-matter physics, on the other hand, the asymptotic condition is not satisfied for electrons in metals and doped semiconductors. In fact, elementary excitations (Landau's quasi particles) are accompanied with the backflow, which extends *all over the crystal* [41], in contradiction to the asymptotic condition. Because of this fundamental difficulty, the scattering approaches to mesoscopic conductors replaced the reservoirs with 1d leads in which electrons are free [7,11,34]. Therefore, real reservoirs, in which electrons behave as 2d or 3d interacting electrons, have not been treated by the scattering-theoretical approaches.

3 Combined Use of Microscopic Theory and Thermodynamics [21]

The basic idea of this method is as follows: Since a QWR is a small system, and is most important, it should be treated with a full quantum theory. On the other hand, reservoirs are large systems whose dynamics is complicated, hence it could be treated with thermodynamics (in a wide sense). Utilizing these observations, we shall develop thermodynamical arguments to find the nonequilibrium steady state that is realized when a finite $\Delta\mu$ is applied between the reservoirs. This is the key of this method because when the steady state is found, G (and other observables) can be calculated by straightforward calculations. Although in some cases *formal* calculations can be performed without finding the steady state [12], we stress that such formal theories are incomplete because another theory is required to relate $\Delta\mu$ of such theories with $\Delta\mu$ of the reservoirs, by which G is defined.

An advantage of the present method is that we do not need to find the relation between $\Delta\phi_{\rm ext}$ and $\Delta\mu$ because $\langle I\rangle$ is directly calculated as a function of $\Delta\mu$. Another advantage is that it is applicable to NEN and nonlinear responses because nonequilibrium steady state is directly obtained.

3.1 Conductance of the 1d Fermi Liquid

It is generally believed that a 1d interacting electron system is not the Fermi liquid (FL) [41], but the Tomonaga-Luttinger liquid (TLL) [16–19]. For this reason, many papers on 1d systems [3–6,8,9,11,12] use the word FL to indicate *non-interacting* electrons, i.e., a Fermi *gas*. However, we do not use such a misleading terminology; by a FL we mean *interacting* quasi-particles. Since the backflow is induced by the interaction [41], the Landauer's argument of non-interacting particles [14] cannot be applied to a FL. On the other hand, real systems have finite length and finite intersubband energies, in contradiction to the assumptions of the TLL. Hence, some real systems might be well described as a FL. Therefore, G of a FL is non-trivial and interesting [15]. Furthermore, we will show in section 5 that the results for the FL suggest very important phenomena that is characteristic to nonequilibrium states of inhomogeneous systems. Note also that the following calculations look similar to the derivation of fundamental relations in the theory of the FL [41]. However, G of mesoscopic conductors was not calculated in such calculations. The most important point to evaluate G is to find the nonequilibrium steady state.

We find the nonequilibrium steady state using a thermodynamical argument as follows: In the reservoirs, electrons behave as a 2d or 3d (depending on the thickness of the reservoir regions) FL. Since we have assumed that $u^{\rm c}$ is smooth and slowly-varying, a 2d or 3d quasi-particle in a reservoir, *together with its backflow*, can evolve adiabatically into a 1d quasi-particle and its backflow in the QWR, without reflection. In this adiabatic evolution, the quasi-particle mass m^* and the Landau parameters f also evolve adiabatically, and the energy is conserved. Therefore, quasi-particles with $\varepsilon(k > 0) \leq \mu_{\rm L}$ are injected from the left reservoir. Here, ε is the quasi-particle energy;

$$\varepsilon(k) = \frac{\hbar^2 k^2}{2m^*} + \frac{\hbar}{\mathcal{L}} \sum_{k'} f(k,k') \delta n(k'), \tag{6}$$

where $\delta n(k) \equiv n(k) - \Theta(|k| \leq k_{\rm F})$, with $n(k)$ being the quasi-particle distribution. The last term of this expression represents energy correction by interactions among quasi-particles [41]. On the other hand, a quasi-hole below $\mu_{\rm L}$ should not be injected because otherwise the recombination of a quasi-particle with the quasi-hole would produce excess entropy, in contradiction with the principle of minimum entropy production. Similarly, quasi-particles with $\varepsilon(k < 0) \leq \mu_{\rm R}$ are injected from the right reservoir, with no quasi-holes are injected below $\mu_{\rm R}$. Therefore, the nonequilibrium steady state under a finite $\Delta\mu = \mu_{\rm L} - \mu_{\rm R}$ should be the "shifted Fermi state", in which quasi-particle states with $\varepsilon(k \geq 0) \leq \mu_{\rm L}$ and $\varepsilon(k < 0) \leq \mu_{\rm R}$ are all occupied. Hence, the right- (left-) going quasi-particles have the chemical potential $\mu_+ = \mu_{\rm L}$ ($\mu_+ = \mu_{\rm R}$). Considering also the charge neutrality, we can write the distribution function as

$$n(k) = \Theta(|k - q| \leq k_{\rm F}). \tag{7}$$