INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

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UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION

Proceedings of the Adriatico Research Conference on

QUANTUM FLUCTUATIONS IN MESOSCOPIC AND MACROSCOPIC SYSTEMS

Editors

H. A. Cerdeira, F. Guinea López and U. Weiss

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H. A. Cerdeira

Universidade Estadual de Campinas, Brazil
and ICTP, Trieste, Italy

F. Guinea López

Universidad Autonoma de Madrid
Instituto de Fisica del Estado Solido (CSIC), Spain

U. Weiss

Universität Stuttgart
Institut für Theoretische Physik II, Germany

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QUANTUM FLUCTUATIONS IN MESOSCOPIC AND MACROSCOPIC SYSTEMS

Foreword

With the rapid advances in microfabrication technology in recent years, physical behaviours that are in between the macroscopic classical picture and the pure quantum nature on the molecular level became increasingly apparent. This regime has been popularized in the field of condensed matter physics as the "mesoscopic" regime. Among the mesoscopic effects that have been observed at low temperatures are a variety of transport phenomena in small metallic samples and semiconductor hetero-structures assigned to quantum coherence, dissipative influences in macroscopic systems ranging from Josephson devices to interstitials in metals, and tunneling phenomena of single electrons and Cooper pairs in small capacitance junctions and junction arrays. The importance of quantum fluctuations in the understanding of such systems is now well established.

The objective of this Adriatico Research Conference was to bring together physicists working in the various sub-fields of mesoscopic physics and to review the status of research in this rapidly developing field with emphasis on current advances and future possibilities. The Conference covered a wide spectrum including quantum transport in small samples, macroscopic quantum tunnelling and quantum coherence, charging effects in tunnel junctions, and correlated charge transfer and quantum vortices in junction arrays. Experimental review talks were given in each of these fields. The emphasis, however, was put on the theoretical understanding of the new phenomena observed. The authors were asked to ensure that their contributions were at a level which would be accessible to graduate students and to non-specialists in their field. This volume should therefore be of use to all those whose work impinges on any part of mesoscopic physics.

It is a pleasure to thank Mrs. Milena Poropat who helped us in the organisation of the Conference and in the completion of this book. We are particularly grateful to ICTP, SISSA and IBM for their financial help.

The Editors.

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I

QUANTUM TRANSPORT

QUANTUM THEORY OF TRANSPORT IN MESOSCOPIC SYSTEMS

Bernhard Kramer
Physikalisch-Technische Bundesanstalt
Bundesallee 100, 3300 Braunschweig, F. R. Germany
and
Jan Mašek
Institute of Physics, Czechoslovak Academy of Sciences
Na Slovance 2, 180 40 Prague, Czechoslovakia

Abstract

The linear response theory for the electrical AC-conductance of mesoscopic systems is formulated, and applied to quasi-one dimensional quantum wires. The influence of disorder on the average of the conductance is discussed. The transition from non-universal to universal conductance fluctuations with increasing disorder is studied. Several predictions concerning the frequency dependence of the conductance and its statistical properties are made. The role of phase breaking processes is investigated.

1 Introduction

In classical (linear) transport theory the electrical behavior of a system can be characterized by the electrical conductivity that depends on various internal and external system parameters

$$\sigma = \sigma(\omega, T, B, E_F, W \cdots) \tag{1}$$

(ω frequency, T temperature, B magnetic field, E_F Fermi energy, W disorder), but is independent of the geometry. Surface and boundary effects are completely neglected. The relation between the total current and the voltage is given by Ohm's law, $I = \Gamma U$, where Γ is the electrical conductance related to the conductivity by the simple geometrical relation

$$\Gamma = \sigma A/L \tag{2}$$

where A and L are the cross-sectional area perpendicular, and the length of the system parallel to the current, respectiviely. In order to obtain the conductivity a microscopic theory is needed. The simplest is the well-known Drude approach which essentially replaces the conductivity by a relaxation time τ. Its validity is restricted to metallic systems where the electron density is high and the electrons are scattered many times within the bulk.

At low temperatures inelastic (phase randomizing) processes, due to electron-phonon scattering, for instance, are frozen out. The inelastic scattering time τ_i becomes large. The mean free path between two inelastic scatterings can exceed the sample size L. In this regime the transport is governed by the quantum states in the system as a whol As a consequence, the electrical transport properties of small conductors exhibit a ri variety of quantum phenomena [1]. They are related to the *coherence* of the electron stat throughout the whole sample, to their *statistical* nature induced by the disorder, and finite size *quantization* . For the theoretical description of these *mesoscopic effects* o needs (i) information about the single particle quantum states in finite, but not atomic(! systems in the presence of disorder, (ii) a suitable transport theory that includes the effe of contacts and leads, and (iii) a theory that allows to include the influence of interactio on the states, and on the transport processes.

The theory of the single particle states is comparatively simple. It requires essential the solution of a Schrödinger equation under certain boundary conditions. By mea of modern computational facilities this is possible even in the presence of disorder f surprisingly large system sizes [2].

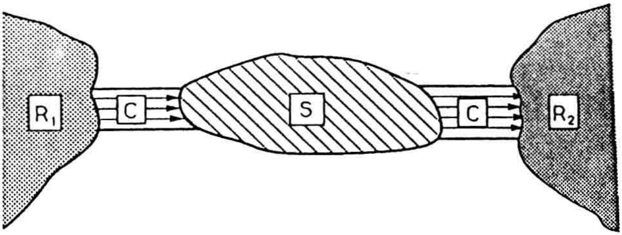
More complicated is the development of the transport theory. Two approaches ha been considered. Most important was the discovery that in the quantum coherent regin the transport properties of a sample must be characterized by size and shape depende conductances or resistances, instead of using the geometry independent components of local, size and shape-independent conductivity or resistivity tensor. It was Landauer [3 who first pointed out in the context of one-dimensional (1 D) disordered conductors th in the DC-limit coherent transport can be related to quantum mechanical transmissio In his approach, phase randomization is excluded completely from the "sample" whic is considered as only a part of a larger system containing in addition "reservoirs", an "ideal leads" that connect the "reservoirs" with the "sample" (Fig. 1). The former a characterized by their chemical potentials and simulate the "world" behind the contact The driving forces for the currents are the differences in the chemical potentials. A inelastic and phase randomizing processes necessary for energy and phase relaxation a incorporated into the "reservoirs" . The (random) potential that represents the "sampl scatters the electrons only elastically. Landauer's approach has not only been conceptuall extremely useful. In addition, it provided an excellent scheme for the explanation of t transport features of 2 D ballistic point contacts, and certain aspects of the quantized Ha effect [4].

On the other hand, quantum mechanical linear response theory relates the local curre density $\vec{j}$, and the electric field $\vec{E}$ via the non-local conductivity tensor (Fig. 2).

$$\vec{j}(\vec{r},t)=\int d^3r'dt'\sigma(\vec{r},t;\vec{r}\,',t')\vec{E}(\vec{r}\,',t')$$

Together with a suitable Hamiltonian Equ. (3) should be able to provide the gener microscopic framework for the quantum transport theory of coherent systems. Thu the Landauer theory, since it is linear, must follow from linear response for the prop geometry as a special limiting case. In the DC-limit the conditions for the equivalen was discussed by several authors [5, 6, 7, 8, 9, 10, 11]. We will not repeat here the vario arguments. We only mention a few facts that strongly motivate the reformulation [12, 13 and the application, of linear response theory for mesoscopic, i.e. quantum coherent b macroscopic systems.

Since it starts from time-dependent currents and fields it can be used for systemat studies of frequency and time dependencies. As a microscopic theory it allows, at least i



'igure 1: Disordered sample of arbitrary shape connected to ideal leads. The leads serve ɔ define the "transport channels" (C). Within the sample (S), the transport channels are ıixed with each other via the scattering induced by the disorder. In the Landauer theory ; is assumed that the chemical potentials μ_i differ in the reservoirs (R_1,R_2) attached to he left and to the right hand sides of the sample via the leads.

ırinciple, to discuss the influence of all of the scattering processes (inelastic and elastic) ın an equal (microscopic) footing. It provides the framework for the identification of he "transport channels" in the Landauer theory. The quantum mechanical transmission ırobability amplitudes of the channels can be calculated microscopically. In addition it an straightforwardly be generalized to discuss non-linear mesoscopic effects [14, 15].

Most difficult is the inclusion of the phase and energy randomizing processes. Although hey can be treated microscopically, in principle, for instance by diagrammatic techniques 16], it turned out to be extremely complicated in practice. For most purposes it suffices o consider these processes to be incorporated into an *inelastic scattering time* τ_{in} that lepends on the temperature[16, 17, 18]. If the temperature is low enough such that this mean time between two successive inelastic events" is of the order of or larger than he characteristic travelling time of an electron through the sample, quantum transport ıhenomena will become experimentally accessible.

In this paper, we want to reformulate the linear response theory for the *time-dependent* ransport in quantum mechanically coherent systems. First we consider the zero tempera- ıre limit, and neglect phase and energy randomization completely. Results for a quasi-1 D tem are reported. On the one hand, they provide insight into the microscopic nature of "transport channels" discussed in the context of the Landauer approach, and, on the r hand, they allow for some predictions concerning the frequency dependence of the onductance for systems without and with a perturbing (random) potential. In a simple nodel we shall also consider the influence of phase randomization.

2 Linear Response for AC-Conductance

The linear response expression for the conductance is obtained straightforwardly in the ısual way. Startpoint is the Hamiltonian

$$\mathbf{H} = \mathbf{H}_0 - \int d^3\vec{r}\vec{A}(\vec{r},t)\vec{\mathbf{j}}(\vec{r}). \tag{4}$$

The influence of the (inhomogeneous) electric field is included linearly via the vector poten- ial, $\vec{E}(\vec{r},t) = \partial\vec{A}/\partial t$. The current density operator is defined as $\mathbf{j} = (e/2m)[\mathbf{p},\delta(\vec{r}-\vec{\mathbf{r}})]_+$,

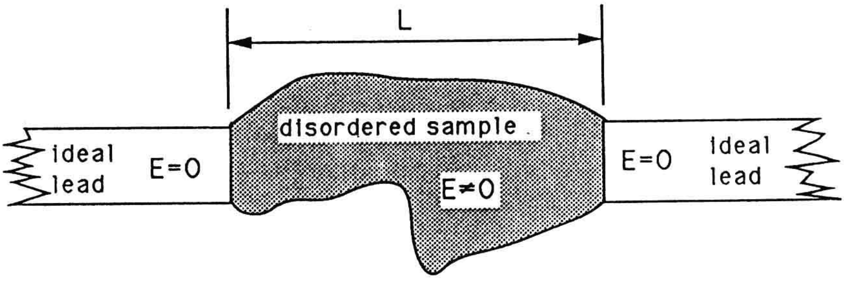


Figure 2: Disordered sample of arbitrary shape connected to ideal, quasi-1 D leads. The sample may be represented by a potential that includes not only the "internal" disorder due to impurities, for instance, but also the geometrical shape. The leads are assumed to be ideal quasi-1 D far away from the sample, not containing any randomness, and to have some finite, asymptotically constant cross-section. They serve to define the "transport channels" that can be shown to be related to the asymptotically free, geometrically quantized quasi-1 D electron states. In the linear response theory it is assumed that the electric field is non-zero only within the sample.

$\mathbf{p} = -i\hbar\partial_x$. For a monochromatic field the vector potential is

$$\vec{A}(\vec{r},t) = \frac{i}{\omega + i\eta}\vec{E}(\vec{r})e^{-i(\omega+i\eta)t} \tag{5}$$

The small imaginary part of the frequency, $i\eta$, guarantees the vanishing of the electric field for $t \to -\infty$. The dissipative conductance $\Gamma(\omega)$, in units of e^2/h, is defined by the absorbed power

$$P(\omega) = \frac{1}{2}\int d^3\vec{r}\,\vec{j}(\vec{r})\cdot\vec{E}(\vec{r}) \equiv \frac{e^2}{2h}\Gamma(\omega)U^2 \tag{6}$$

where $U = \int d\vec{r}\cdot\vec{E}(\vec{r})$ is the applied voltage. Calculating the current density as a function of the electric field in linear approximation one obtains the conductivity as

$$\sigma(\omega;\vec{r},\vec{r}\,') = \int dE\,\frac{f(E) - f(E+\hbar\omega)}{\hbar\omega}\,\sigma_0(E;\vec{r},\vec{r}\,') \tag{7}$$

where $f(E)$ is the Fermi distribution function, and

$$\sigma_0(E;\vec{r},\vec{r}\,') \equiv \hbar Tr\{\delta(E+\hbar\omega - \mathbf{H_0})\vec{\mathbf{j}}(\vec{r}\,')\delta(E - \mathbf{H_0})\vec{\mathbf{j}}(\vec{r})\} \tag{8}$$

is the conductivity tensor at $T = 0$. Using Equ.'s (6) and (7) the conductance is obtained from

$$\Gamma(\omega) = \frac{h}{e^2U^2}\int d^3\vec{r}\int d^3\vec{r}\,'\vec{E}(\vec{r})\cdot\sigma(\omega;\vec{r},\vec{r}\,')\cdot\vec{E}(\vec{r}\,') \tag{9}$$

Assuming that the electric field is homogeneous within a certain region Ω of the length L in the direction of $\vec{E}$, say the x-direction, we obtain

$$\Gamma(\omega) = \frac{h}{e^2L^2}\int_\Omega d^3\vec{r}\int_\Omega d^3\vec{r}\,'\sigma(\omega;\vec{r},\vec{r}\,') \tag{10}$$

In general, the AC-conductance depends on the spatial behavior of the electric field. It is only in the DC-limit where it can be defined independent of the field due to current conservation in the leads [5, 7]. The well-known result for a sample connected with two leads is

$$\Gamma(0) = \left(\frac{\hbar k}{m}\right)^2 \lim_{x,x' \to \infty} Tr\{|G^+(E;x,x')|^2\} \tag{11}$$

where E is the Fermi energy, k the wave vector of the asymptotically free states in the leads at the Fermi energy, and $\mathbf{G} \equiv (z - \mathbf{H_0})^{-1}$ the one-electron Green's function subject to free boundary conditions for $x, x' \to \infty$. The trace is taken over the (asymptotically free) states at the Fermi energy that are characterized by k. They correspond to the transport channels in the Landauer theory. Generalizations to the multi-lead case can be found in [12, 13].

In order to proceed with the evaluation of the frequency dependence it is necessary to discuss the properties of the eigenfunctions of $\mathbf{H_0}$ in more detail.

3 AC-Conductance of Quantum Wires

Some of the most important properties of quantum AC-transport become transparent when we consider independent electrons in an ideal "quantum wire" of the length $L\ (\to \infty)$ in the x-direction (periodic boundary conditions), and of a constant finite width M in the perpendicular directions. The "sample" can then be defined by adding to the Hamiltonian an additional potential that describes the influence of the impurities, and of the geometrical shape. Without potential we consider the portion of the quantum wire containing the applied electric field as the "sample". The eigenvalues and eigenstates of the Schrödinger equation for the ideal quantum wire are

$$E_\mu(k) = E_\mu + \frac{\hbar^2 k^2}{2m}, \tag{12}$$

$$\Psi_{\mu k} = \phi_\mu(y,z) e^{ikx}. \tag{13}$$

Due to the geometrical constriction of the motion of the electrons perpendicular to the x-direction the spectrum consists of well separated quasi-1 D energy bands. In the presence of a periodic potential which may be taken into account by using a tight binding Hamiltonian with nearest neighbor coupling matrix element V, the general structure of the spectrum and the wave functions is the same. However, in this case $\hbar^2 k^2/2m$ has to be replaced by $2V \cos k$, and e^{ikx} by $\sum_j e^{ikj}\langle x|j\rangle$ where $|j\rangle$ are the states associated with the lattice sites.

In the presence of a magnetic field the motions in the x- and in the perpendicular directions do no longer decouple. The shape of the energy bands and the corresponding wave functions are more complicated, although the changes remain small as long as the cyclotron energy is small compared with the distance between two successive energy bands (Fig. 3). A moderate perturbing potential (disorder, boundaries) introduces strong mixing of the bands apparent near the onsets E_μ due to the associated van Hove singularities in the density of states [19, 20, 21]. As mentioned above, the quasi-1 D subbands define the "transport channels" occurring in the Landauer approach: at zero temperature transport takes place only in states with wave-vectors that correspond to intersections of the band

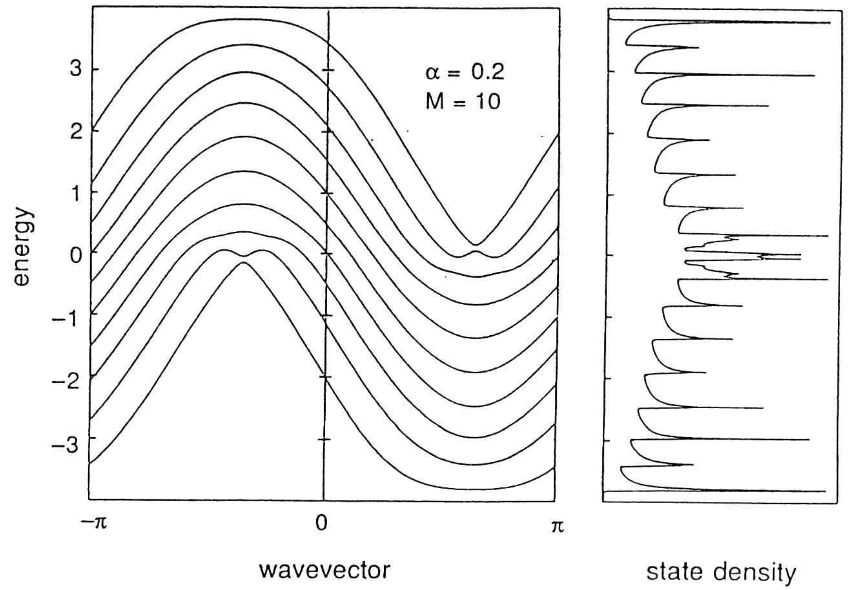


Figure 3: Quasi-1 D energy bands (in units of V, the nearest neighbor matrix element of the Hamiltonian) of a tight binding system of the width M in the presence of a perpendicular magnetic field of the strength $B = \alpha\phi_0$ (ϕ_0 magnetic flux quantum).

structure $E_\mu(k)$ with the Fermi energy E_F. A given 1 D subband may correspond to several channels depending on its shape (Fig. 3).

For Bloch waves in the x-direction (ideal system without perturbing potential) the non-local conductivity may be evaluated explicitly [23]. The frequency dependent conductance is given by the Fourier transform of the auto-correlation function of the field, $L(q) = \int dx dx' E(x)E(x+x')e^{iqx'}$.

$$\Gamma(\omega) = \sum_{\mu=1}^{\mu_{occ}} \frac{L(\omega/v_\mu)}{L(0)} \tag{14}$$

$v_\mu = [2(E_F - E_\mu)/m]^{1/2}$ is the Fermi velocity in the μth subband. μ_{occ} is the total number of the occupied channels.

The linear response expression for the conductance of a coherent quasi-1 D quantum system shows several interesting general features that are very important for the understanding of the experiments [19, 20, 21, 23, 24, 25, 27].

1. For an ideal system (without perturbing potential) the conductance may be written as a sum of the contributions of independent transport channels. This remains true even in the presence of a homogeneous magnetic field.

2. The single contributions to the conductance of the individual subbands scale as $(\sin(x)/x)^2$, $x = \omega L/2v_\mu$, if the electric field is assumed to be homogeneous within

an interval of the length L and zero outside.

3. In general the conductivity tensor is non-local in space and time. The conductance depends on the geometry in a non-trivial way. For instance, not only narrowing but also widening of a system locally may decrease its conductance in the coherent regime.

4. The AC-conductance depends on the spatial shape of the electric field (Fig. 4). In order to predict the result of an experiment one would have to know the spatial dependence of the field in the sample, i. e. one would have to consider interaction effects and screening.

5. In the DC-limit only the applied voltage is of importance. For the ideal quasi-1 D system the DC-conductance is quantized and given by $(e^2/h)\mu_{occ}$ independent of the length of the system, and of the spatial behavior of the electric field (Fig. 5). This shows explicitely the equivalence of the Landauer theory to linear response in the DC-limit since the single channel transmission probabilities are equal to one without inter-channel scattering and disorder.

4 Influence of a Perturbing Potential on DC Transport

Perturbing potentials may have various physical origins. Impurities, defects, dislocations, and surface roughness lead unavoidably to a certain degree of disorder in any real sample. Also the man-made shape of a sample may be represented by some additional potential energy. In order to compare with experiments it is necessary to study the influence of these perturbations on the conductance. Here we consider only the case of a random potential.

Figure 6 shows the average of the DC-conductance as a function of the Fermi energy of a quasi-1 D tight binding system subject to a random potential energy that is distributed according to a box distribution of a width W [20]. The average conductance is still quantized, although the unit of quantization (heights of the steps) is smaller than e^2/h. Due to the disorder, the conductance fluctuates within the statistical ensemble. The square root of the variance (rms) of the conductance fluctuations, $\Delta\Gamma$, are shown as vertical bars in the figure. As can be seen from the insert, approximate quantization persists as long as $\Delta\Gamma$ does not exceed the average step height which happens here at $W = V$ (V is the off-diagonal matrix element of the Hamiltonian between nearest neighbor lattice sites). At the onset of each of the plateaus one observes a sharp anti-resonance like quenching of the conductance which can be attributed to an enhancement of the impurity scattering due to the van Hove singularities in the density of states at the onsets of the 1 D subbands. The width of the anti-resonances increases with increasing disorder and length of the sample. instead of quantized plateaus the conductance shows a non-monotonous increase with regular oscillations. The effect predicted in [20, 21, 22] has been observed in recent experiments on narrow constrictions prepared on materials with lower mobility [25, 26].

The behavior of the fluctuations of the conductance is shown in more detail in Fig. 6 where we have plotted $rms(\Gamma)$ of a tight binding system with randomness W, of the width M, and of the length L for different Fermi energies as a function of $W\sqrt{L}$ [27]. First of all, we observe that $rms(\Gamma)$ scales as a function of $W\sqrt{L}$. Secondly, for $W\sqrt{L} \leq 2$,

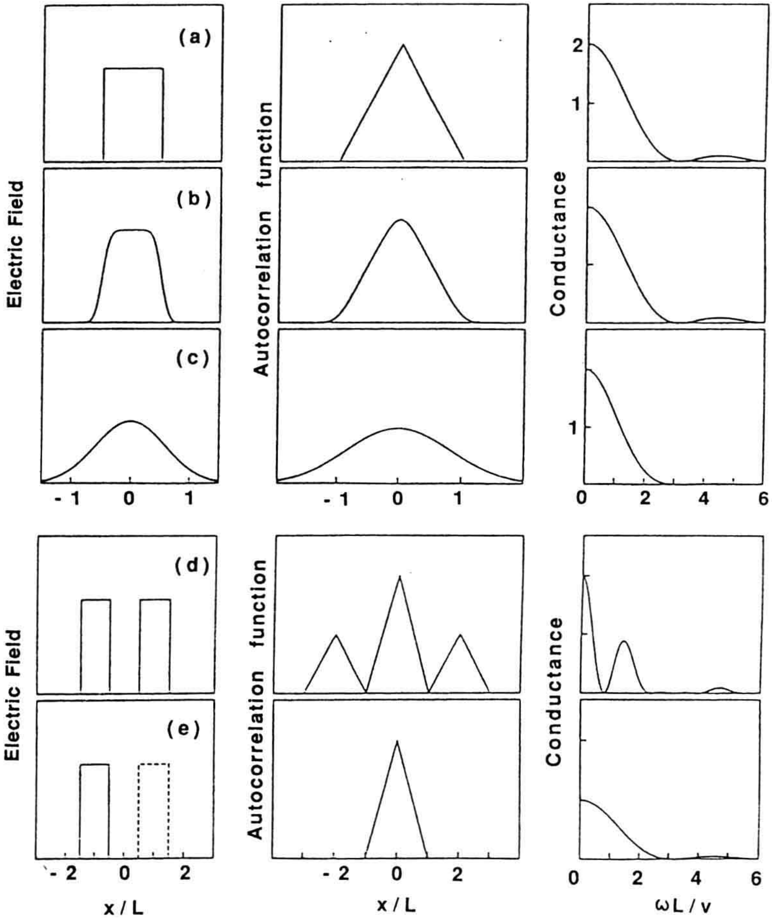


Figure 4: Spatial dependence of the electric field (left), auto-correlation function (middle), and the corresponding frequency dependence of the conductance (right). In model (d) it was assumed that the states within the two intervals of non-vanishing electric field are coherent, whereas in case (e) they were incoherent.