

Unified description of coherent and dissipative electron transport

K. Maschke

Institut de Physique Appliquée, Ecole Polytechnique Fédérale, Lausanne, Switzerland

M. Schreiber

Institut für Physikalische Chemie, Johannes-Gutenberg-Universität, 6500 Mainz, Federal Republic of Germany

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We apply the Landauer-Büttiker theory of dc electron transport to a chain of scatterers, which are coupled to an external heat bath. In this approach, coherent and dissipative transport are treated in a unified manner, and the suppression of quantum coherence effects for increasing coupling with the heat bath can be described. In particular, we find that the resonant behavior of the conductance with respect to the Fermi wave vector disappears gradually with increasing coupling. For intermediate coupling, resonance effects are only found for sufficiently small samples. They disappear asymptotically with increasing sample size. The characteristic length for this dephasing effect corresponds to the mean free path, which is derived from the exponential decay of the transmission coefficient in the presence of inelastic scattering.

I. INTRODUCTION

Interference effects due to coherent transport have been observed in mesoscopic systems with and without magnetic field. These phenomena can be described in a very efficient manner by the Landauer theory of coherent transport,¹ which relates the conductance of the considered system to its scattering properties. The influence of inelastic scattering on the observed interference phenomena like Aharonov-Bohm oscillations,² conductance fluctuations,^{3,4} or persistent currents⁵ has become an important issue. In his original work Landauer has in particular investigated the influence of elastic scattering on the electron transport. Nevertheless, he noticed immediately that in an open system inelastic phase-breaking processes will destroy the quantum coherence and thus lead to dissipative electron transport. This idea has been pursued by several authors. In an explicit manner, Büttiker introduced dissipation in a small normal-metal loop by attaching the loop via a single lead to an electron reservoir.⁶ This approach has been developed during the last few years by Büttiker as well as several other authors.⁷⁻¹⁵ In particular, it has been used with great success for the interpretation of multiprobe experiments.⁷⁻¹³ Most recently, D'Amato *et al.*¹⁴ have discussed the conductance of ordered and disordered chains in the presence of inelastic scattering, where the scattering probabilities are calculated with a Green's-function method. Datta¹⁵ has shown that the Landauer-Büttiker approach is consistent with a quantum-mechanical description of dissipation by the interaction of electrons with a reservoir of independent harmonic oscillators.

In the present paper we apply the Landauer-Büttiker theory to a chain of scatterers with elastic as well as inelastic scattering channels. In the absence of inelastic scattering the multiple scattering of the electron states

with Fermi wave vector q leads to pronounced quantum-coherence effects. Following Büttiker,^{6,7,9,11} we introduce a scattering matrix which not only accounts for elastic scattering within the transport channels but also for scattering from the transport channels into side channels. The side channels connect the sample to its environment which is represented by a local heat bath or electron reservoir. Electrons entering the heat bath are reinjected into the sample with an arbitrary phase. The scattering involving the heat-bath channels thus gives rise to irreversible dephasing. We emphasize that the heat-bath channels are introduced to describe open systems, i.e., their presence does not necessarily imply that we add voltage probes to the chain. This would only be adequate for the discussion of multiprobe measurements. In other words, we consider open systems, in which the electrons everywhere within the sample are coupled with the local environment. Depending on the considered specific system, the coupling may depend on the spatial position.

The transformation of the scattering matrices into transfer matrices enables us to connect the scatterers in a straightforward way. For a realistic model of a one-dimensional conductor between ideal contacts, we consider a finite chain of scatterers and derive its scattering matrix from the overall transfer matrix. The local chemical potential for the heat bath at each scatterer is determined from the current conservation conditions. The resistance can then be calculated in terms of the chemical potentials and the interchannel transition probabilities which follow from the total scattering matrix of the chain. As in the original formulation of Landauer for the fully elastic case of an isolated chain with open ends at the contacts, the resistance of the sample can be defined in terms of its scattering properties. As an example, we use this approach to investigate the influence of irreversible processes on quantum coherence in a chain of identical scatterers.

II. MODEL OF THE GENERALIZED SCATTERER

We describe the single scatterers by their scattering matrices, which relate the incoming waves to the outgoing waves. In the case of a single elastic scatterer, we have to consider two transport channels, 1 and 2. If we denote the coefficients of the incoming waves in channel i by c_i and of the respective outgoing waves by c'_i , we obtain

$$\begin{pmatrix} c'_1 \\ c'_2 \end{pmatrix} = \underline{\sigma} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}, \quad (1)$$

where $\underline{\sigma}$ is the scattering matrix of a single elastic scatterer. For simplicity we suppose the scatterer to be symmetric. Then it can be described in terms of the reflection coefficient r and the transmission coefficient t . If we place the scatterer at the origin, its scattering matrix is

$$\underline{\sigma} = \begin{pmatrix} r & t \\ t & r \end{pmatrix}, \quad (2)$$

which must be unitary, so that

$$|r|^2 + |t|^2 = 1. \quad (3)$$

In this paper we neglect any wave-vector or energy dependence of r and t . For our present purposes it is sufficient to use the simple parametrization

$$\begin{aligned} r &= i\sqrt{1-\delta}, \\ t &= \sqrt{\delta}. \end{aligned} \quad (4)$$

We now introduce a generalized scatterer which allows for reversible elastic as well as for irreversible inelastic scattering. In addition to the two channels for the transport, this requires two more channels⁸ towards the heat bath (channels $2n+1$ and $2n+2$ in Fig. 1). Assuming that the scatterer is placed at the origin, we define the corresponding scattering matrix by

$$\underline{s}_0 = \begin{pmatrix} ar & at & 0 & \beta \\ at & ar & \beta & 0 \\ 0 & \beta & ar & -at \\ \beta & 0 & -at & ar \end{pmatrix} = \begin{pmatrix} \alpha\underline{\sigma} & \beta\underline{\mathbb{1}} \\ \beta\underline{\mathbb{1}} & \alpha\underline{\sigma} \end{pmatrix}. \quad (5)$$

The submatrices $\beta\underline{\mathbb{1}}$ with

$$\underline{\mathbb{1}} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (6)$$

couple the elastic channels with the heat bath. The relative strength of elastic and inelastic scattering is given by the parameters

$$\begin{aligned} \alpha &= \sqrt{1-\varepsilon}, \\ \beta &= \sqrt{\varepsilon}. \end{aligned} \quad (7)$$

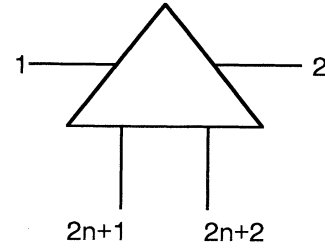


FIG. 1. Channels of a single scatterer at position n . Coupling with the heat bath: channels $2n+1$ and $2n+2$. Transport channels: 1,2.

Thus $\varepsilon=0$ corresponds to a completely elastic scatterer and $\varepsilon=1$ to a completely inelastic scatterer. The scattering within the heat bath, which is described by $\alpha\underline{\sigma}$ with

$$\underline{\sigma} = \begin{pmatrix} r & -t \\ -t & r \end{pmatrix}, \quad (8)$$

is necessary in order to obtain a unitary scattering matrix.

The incoming and outgoing wave functions obey the translation symmetry of Bloch waves. It follows that a displacement of the scatterer from the origin to a position na , where a is the lattice constant, leaves the transmission coefficient unchanged, whereas the reflection coefficient is changed by a phase factor. For the reflection in channels 1 and 2, we get

$$\begin{aligned} r_{1n} &= r e^{-2iqna}, \\ r_{2n} &= r e^{2iqna}. \end{aligned} \quad (9)$$

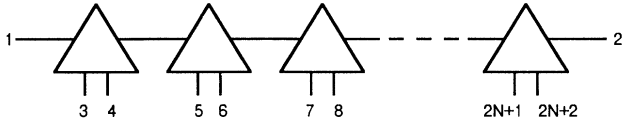
For zero temperature, q is equal to the Fermi wave vector. The corresponding scattering matrix becomes

$$\underline{s}_n = \begin{pmatrix} \alpha\underline{\sigma}_n & \beta\underline{\mathbb{1}} \\ \beta\underline{\mathbb{1}} & \alpha\underline{\sigma}_n \end{pmatrix}, \quad (10)$$

where $\underline{\sigma}_n$ and $\underline{\sigma}_n$ are defined in accordance with Eqs. (2) and (8) replacing r by r_{1n} and r_{2n} .

III. CONSTRUCTION OF THE SCATTERING MATRIX OF A CHAIN OF SCATTERERS

For the case of N scatterers within the chain, the dimensions of the scattering matrix of the whole chain as well as that of a single scatterer are given by the total number of channels within the chain, which is equal to $2N+2 \equiv M$ (see Fig. 2). If we order the channels as indicated in Fig. 2, the scattering matrix of the single scatterer at the n th position becomes

FIG. 2. Chain of N scatterers. The labels count the channels.

$$\underline{S}_n = \begin{pmatrix} \alpha \underline{a}_n & \underline{0} & \cdots & \beta \underline{\bar{1}} & \cdots & \underline{0} \\ \underline{0} & \underline{\bar{1}} & \cdots & \underline{0} & \cdots & \underline{0} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ \beta \underline{\bar{1}} & \underline{0} & \cdots & \alpha \underline{\bar{a}}_n & \cdots & \underline{0} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ \underline{0} & \underline{0} & \cdots & \underline{0} & \cdots & \underline{\bar{1}} \end{pmatrix}. \quad (11)$$

We note that the channels to the heat bath at locations other than na are decoupled from the rest.

We are now in a position to construct the scattering matrix of a chain of N scatterers. We first have to transform the scattering matrices (11) into the corresponding transfer matrices of the single scatterers. This transformation can be derived from the respective definitions: The scattering matrices relate the outgoing to the incoming waves, i.e.,

$$\begin{pmatrix} c'_1 \\ c'_2 \\ \vdots \\ c'_{M-1} \\ c'_M \end{pmatrix} = \underline{S}_n \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_{M-1} \\ c_M \end{pmatrix}. \quad (12)$$

For the definition of the transfer matrices \underline{T}_n we have to distinguish between the waves in the right channels ($2, 4, \dots, M$) and left channels ($1, 3, \dots, M-1$):

$$\begin{pmatrix} c'_2 \\ c_2 \\ \vdots \\ c'_M \\ c_M \end{pmatrix} = \underline{T}_n \begin{pmatrix} c_1 \\ c'_1 \\ \vdots \\ c_{M-1} \\ c'_{M-1} \end{pmatrix}. \quad (13)$$

In order to establish the relation between \underline{S}_n and \underline{T}_n , we consider Eq. (12) for the M special cases in which only one channel carries an incoming wave, and determine the coefficient vectors of the outgoing waves. Inserting all coefficients into Eq. (13) yields the matrix equation

$$\underline{A}_n = \underline{T}_n \underline{B}_n, \quad (14)$$

with

$$\underline{A}_n = \begin{pmatrix} S_{21}^n & S_{22}^n & S_{23}^n & S_{24}^n & \cdots & S_{2M}^n \\ 0 & 1 & 0 & 0 & \cdots & 0 \\ S_{41}^n & S_{42}^n & S_{43}^n & S_{44}^n & \cdots & S_{4M}^n \\ 0 & 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 \end{pmatrix}, \quad (15)$$

where the S_{ij}^n are the matrix elements of the matrix \underline{S}_n and

$$\underline{B}_n = \begin{pmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ S_{11}^n & S_{12}^n & S_{13}^n & S_{14}^n & \cdots & S_{1M}^n \\ 0 & 0 & 1 & 0 & \cdots & 0 \\ S_{31}^n & S_{32}^n & S_{33}^n & S_{34}^n & \cdots & S_{3M}^n \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ S_{M-1,1}^n & S_{M-1,2}^n & S_{M-1,3}^n & S_{M-1,4}^n & \cdots & S_{M-1,M}^n \end{pmatrix}, \quad (16)$$

which has to be inverted to calculate \underline{T}_n from Eq. (14).

The transfer matrix of the system of N scatterers is then given by

$$\underline{T}_{\text{tot}} = \underline{T}_N \underline{T}_{N-1} \cdots \underline{T}_1. \quad (17)$$

Using a similar procedure as for Eq. (14), we obtain the corresponding scattering matrix from

$$\underline{S}_{\text{tot}} \underline{D} = \underline{C}, \quad (18)$$

with

$$\underline{C} = \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots & 0 \\ t_{11} & t_{12} & t_{13} & t_{14} & \cdots & t_{1M} \\ 0 & 0 & 0 & 1 & \cdots & 0 \\ t_{31} & t_{32} & t_{33} & t_{34} & \cdots & t_{3M} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ t_{M-1,1} & t_{M-1,2} & t_{M-1,3} & t_{M-1,4} & \cdots & t_{M-1,M} \end{pmatrix} \quad (19)$$

and

$$\underline{D} = \begin{pmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ t_{21} & t_{22} & t_{23} & t_{24} & \cdots & t_{2M} \\ 0 & 0 & 1 & 0 & \cdots & 0 \\ t_{41} & t_{42} & t_{43} & t_{44} & \cdots & t_{4M} \\ \vdots & \vdots & \vdots & \vdots & \cdots & \vdots \\ t_{M1} & t_{M2} & t_{M3} & t_{M4} & \cdots & t_{MM} \end{pmatrix}, \quad (20)$$

where the t_{ij} are the matrix elements of $\underline{T}_{\text{tot}}$. The scattering probabilities between the various channels are obtained from Eq. (18) as

$$p_{ij} = |s_{ij}|^2, \quad (21)$$

where s_{ij} denotes the matrix elements of $\underline{S}_{\text{tot}}$. In our case we get $p_{ij} = p_{ji}$ due to the symmetry of the single scatterers. We note that the scattering probability p_{12} describes the transmission across the sample.

IV. CALCULATION OF THE RESISTANCE

The resistance of the chain depends on the scattering probabilities p_{ij} as well as on the properties of the heat bath at the scatterers. The latter are specified by the respective chemical potentials μ_i (see Fig. 3) and the temperature T . Here we restrict ourselves to the case $T=0$. For the subsequent discussion we calculate the resistance of the total system, i.e., with included contacts. These are characterized by the chemical potentials μ_1 and μ_2 , as indicated in Fig. 3.

The currents within the different channels can be expressed in terms of the above parameters. Taking into account that only electrons with energies between μ_i and μ_j contribute to the current between channels i and j , we obtain

$$I_i = \frac{e}{h} \sum_{j=1}^M p_{ij} (\mu_i - \mu_j), \quad i = 1, 2, \dots, M, \quad (22)$$

which is the central result of Ref. 9. The prefactor e/h arises from the product between the electron charge, the group velocity, and the density of states at the Fermi energy, which is multiplied by a factor $\frac{1}{2}$ since only electrons traveling in one direction have to be considered for the current.

The chemical potentials are obtained from the conditions of current conservation which read

$$I_{2n+1} + I_{2n+2} = 0. \quad (23)$$

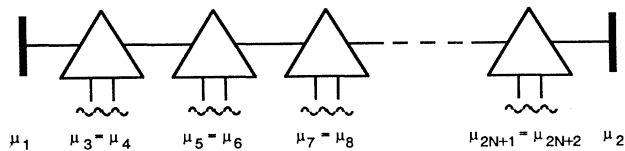


FIG. 3. Chemical potentials in the chain and at the contacts. The indices correspond to the channel labels in Fig. 2. Since each scatterer is connected to a heat bath by two channels, the respective chemical potentials are identical.

If we write the chemical potentials as

$$\mu_{2n+1} = \mu_2 + \chi_n (\mu_1 - \mu_2), \quad n = 1, 2, \dots, N \quad (24)$$

we obtain for the χ_n the following inhomogeneous system of linear equations:

$$W_{n0} \chi_n + \sum_{m=1}^N W_{nm} (\chi_n - \chi_m) = p_{1,2n+1} + p_{1,2n+2}, \quad n = 1, 2, \dots, N \quad (25)$$

with

$$W_{nm} = p_{2n+1,2m+1} + p_{2n+1,2m+2} + p_{2n+2,2m+1} + p_{2n+2,2m+2}. \quad (26)$$

From the solutions χ_n we calculate the chemical potentials, which are inserted into Eq. (22) to determine the currents. In particular, we need the current in the transport channels which is conserved, so that $I_1 = -I_2$. As the voltage difference across the contacts is given by $(\mu_1 - \mu_2)/e$, we obtain for the resistance

$$R = \frac{h}{e^2} \frac{1}{p_{12} + \sum_{n=1}^N \chi_n (p_{2,2n+1} + p_{2,2n+2})}. \quad (27)$$

According to Eq. (25), the χ_n depend only on the scattering matrix of the chain. It follows from Eq. (27) that the same is true for the resistance, in full analogy with the results of Landauer for an elastic chain. A similar relation has been given by D'Amato *et al.*¹⁴ The denominator can be interpreted as an effective transmission probability. It consists of two parts: the contribution of coherent tunneling p_{12} and the incoherent contribution of electrons which were scattered inelastically.

For an ideal lead, i.e., $\delta=1$ and $\epsilon=0$, we have $p_{12}=1$ and $p_{2i}=0$ for $i>2$. In this case Eq. (27) reduces to the contact resistance

$$R_c = h/e^2. \quad (28)$$

In the case of completely elastic scatterers, i.e., $\epsilon=0$ but $\delta \neq 1$, this contact resistance causes the difference between the two Landauer formulas which can be found in the literature. From Eq. (27) we obtain for the two-probe resistance, which includes the contacts,

$$R_2 = \frac{h}{e^2} \frac{1}{p_{12}}. \quad (29)$$

By subtracting the contact resistance, we obtain for the sample resistance

$$R_s = R_2 - R_c = \frac{1 - p_{12}}{p_{12}}. \quad (30)$$

V. DISCUSSION OF THE NUMERICAL RESULTS

In order to illustrate the method, we present in the following the results for a chain of N identical scatterers. This simple case is just chosen for convenience. It is obvious that without any additional difficulties, our method

could equally well be applied to an inhomogeneous chain, in which the scattering properties depend on the position.

Considering Eq. (27) and the subsequent arguments, it can be expected that the resistance of the chain is dominated by the behavior of the transmission probability p_{12} , at least in the limit of small coupling ε to the heat bath. In Fig. 4 we present an example of its dependence on the wave vector q for typical values of the parameters. For vanishing ε the interference effects due to multiple elastic scattering are clearly seen. Increasing inelastic coupling quickly leads to a dephasing of the scattered waves, so that the oscillations in Fig. 4 are strongly damped. Moreover, the overall transmission is reduced in the presence of the inelastic backscattering. It is interesting to note that the transmission probability is very small for extreme values of the wave vector. This behavior can be interpreted as a band-structure effect, corresponding to the occurrence of surface states in a finite chain. The respective range of q values increases with increasing elastic scattering irrespective of the inelastic scattering strength. Accordingly, the q window for significant transmission narrows with decreasing δ .

The same behavior can be deduced from the dependence of the transmission probability on the chain length, as shown in Fig. 5. For large δ , the chosen value of q falls into the discussed transmission window. The fluctuations with N are again a consequence of interference effects which depend, of course, on the number of scatterers. For small δ we are outside the mentioned window, and significant transmission is possible only for short chains. The transmission probabilities decay with increasing number of scatterers.

The influence of inelastic scattering also leads to a decay of the transmission probabilities for increasing chain length. To study this behavior, we analyze the decay length $\lambda(N)$ defined by

$$p_{12}(\varepsilon, N) = p_{12}(\varepsilon=0, N) \exp[-N/\lambda(N)]. \quad (31)$$

If the thus defined decay length converges for large N , its

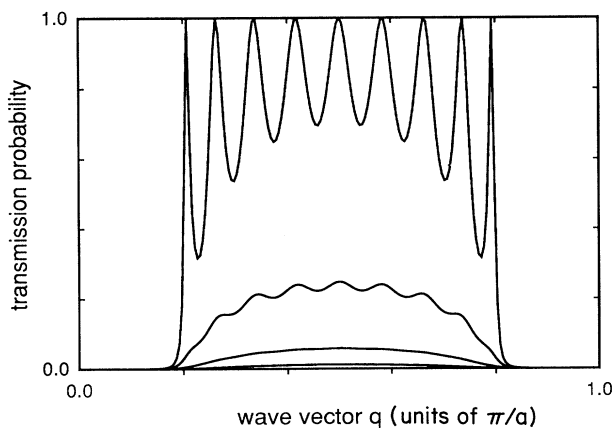


FIG. 4. Transmission probability for a chain of 10 scatterers for inelastic scattering strength $\varepsilon=0, 0.1, 0.2,$ and 0.3 (from top to bottom). The elastic transmission probability for each scatterer is $\delta=0.7$.

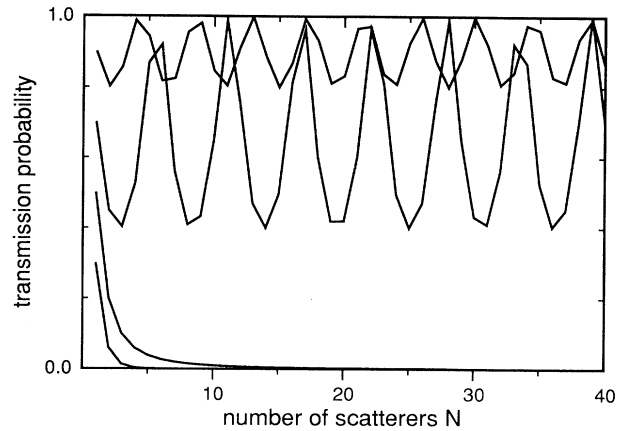


FIG. 5. Transmission probability for a chain of N elastic scatterers ($\varepsilon=0$) at $q=0.25\pi/a$. The transmission probability of each scatterer is $\delta=0.3, 0.5, 0.7,$ and 0.9 (from bottom to top).

limit can be interpreted as the inelastic mean free path. This convergence is shown in Fig. 6. We note that the inelastic mean free path depends also on the elastic scattering, because the effective number of inelastic scattering processes increases with the reflection probability. We have also found a strong wave-vector dependence of the decay length and the mean free path, which could be expected as a consequence of the q dependence of the transmission probability (Fig. 4). It is obvious that the above-discussed interference and dephasing effects will characteristically influence the resistance. This is demonstrated in Fig. 7, where the wave-vector dependence of the resistance is presented. A comparison with Fig. 4 shows that the main features of the resistance are determined by the transmission probability. The other scattering probabilities which enter the relation for the resistance [Eq. (27)] and which involve the side channels do not give rise to any additional oscillations but only reduce the absolute value of R .

With increasing inelastic coupling, the resistance increases for q values within the above-described transmission window and decreases in the regime of the “surface states.” This contrasting behavior can be clearly seen from a comparison of Figs. 8(a) and 8(b) where the dependence of R/N on the chain length is depicted for small and intermediate values of q , respectively. If this quantity converges, its asymptotic value equals the resistivity. It can be seen from Fig. 8 that the length after which this limiting behavior is reached depends strongly on the inelastic coupling, and is of the order of the previously derived mean free path.

VI. CONCLUDING REMARKS

We have demonstrated that the Landauer-Büttiker theory of dc electron transport can easily be applied to a chain of scatterers with elastic and inelastic channels. Starting from Büttiker’s model of separate elastic and inelastic scatterers,⁶ we have introduced a scatterer which comprises elastic and inelastic scattering in such a way

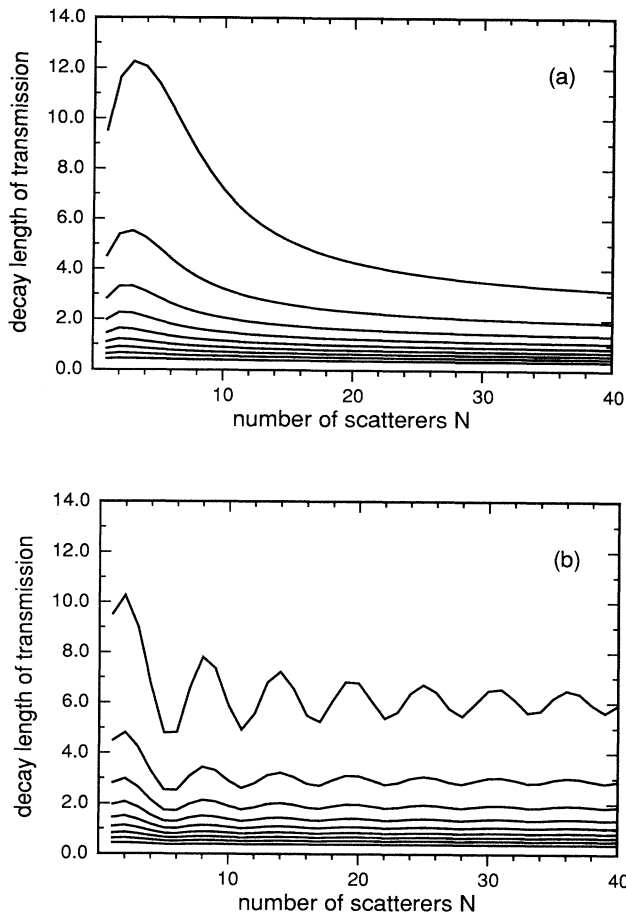


FIG. 6. Decay length (in units of the lattice constant a) of the transmission probability through a chain of N scatterers at $q = 0.25\pi/a$ for $\epsilon = 0.1, 0.2, \dots, 0.9$ (from top to bottom). The elastic transmission probability of each scatterer is (a) $\delta = 0.5$, (b) $\delta = 0.7$.

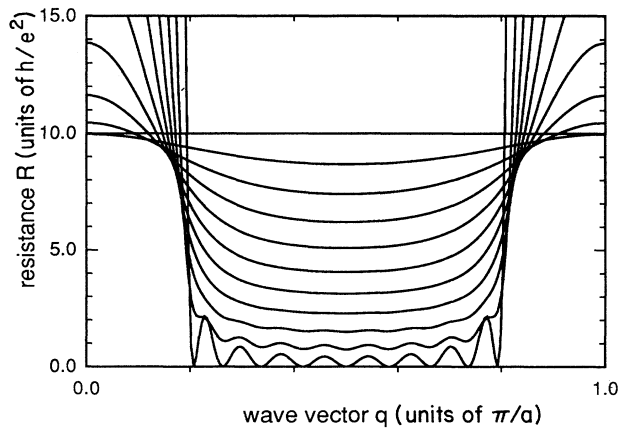


FIG. 7. Resistance of a chain of 10 scatterers for inelastic scattering strengths $\epsilon = 0, 0.1, \dots, 1$ (from bottom to top near the center of the figure). The elastic transmission probability of each scatterer is $\delta = 0.7$. The contact resistance is subtracted.

that the respective parameters cover the whole range of coupling strengths. We have shown how the scattering properties of a chain of these scatterers can be computed. Our formulation leads to a consistent description of both coherent and dissipative transport, which not only explains the essential features of the extreme cases of coherent and dissipative transport, but also describes the delicate interplay between interference and dephasing effects in the intermediate regime. In particular, we have been able to make the following observations.

As expected, the elastic coupling leads to strong interferences due to backscattering. These quantum-coherence effects are gradually suppressed by inelastic processes. The dephasing can be seen, e.g., in the behavior of the transmission probability and the resistance. With respect to their wave-vector dependence, two qualitatively different regimes can be distinguished already in the fully elastic case: Within a certain q window, the size of which decreases with increasing reflection coefficient of the single scatterers, transmission is not attenuated even in the limit of an infinite chain; inelastic scattering

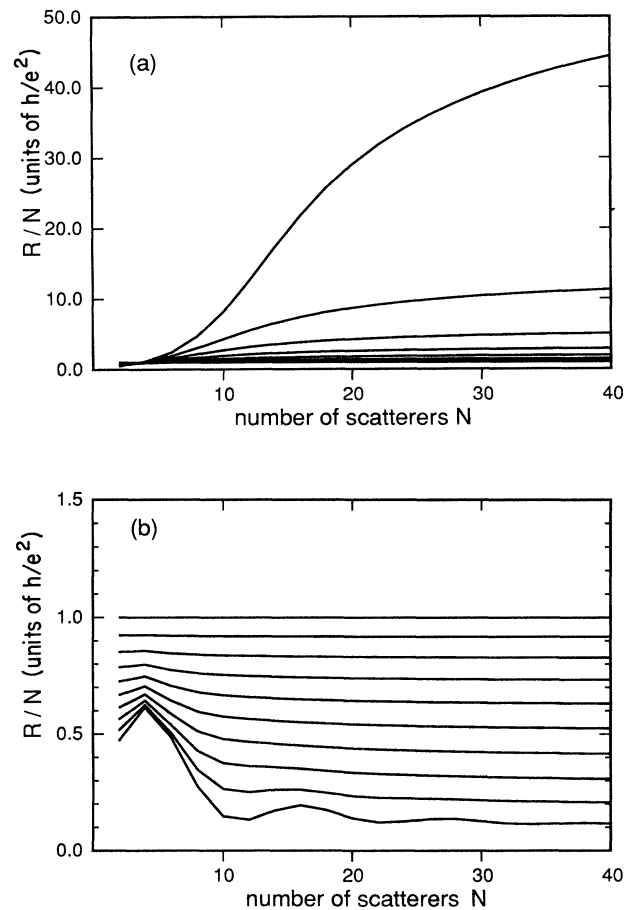


FIG. 8. Resistance of a chain of N scatterers scaled with the chain length N for (a) $q = 0$ and (b) $q = 0.25\pi/a$ and inelastic scattering lengths $\epsilon = 0.1, 0.2, \dots, 1$ [from top to bottom in (a) and vice versa in (b)]. The elastic transmission probability of each scatterer is $\delta = 0.7$.

reduces the transmission probability and accordingly increases the resistance. Outside the window, interference effects are so destructive that the waves can only penetrate over a short length; in this range the weakening of the interference by inelastic scattering increases the transmission probability, and therefore decreases the resistance. The length scale of the dephasing is given by the inelastic mean free path, which is determined from the decay of the transmission probability with the chain length. We note, however, that the thus defined mean free path should not be used to calculate the resistance by

means of the Drude formula, because of the coherent contributions to the transport.

We believe that the method presented will be helpful for the study of a large variety of phase-sensitive transport phenomena. In particular, we intend to investigate the recently discussed oscillations of the chemical potential.¹¹ An interesting extension of the method would be to include disorder either by randomizing the spacing between the scatterers or by choosing a sequence of different scatterers according to some appropriate distribution.

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