

Gauge invariance and absence of exact conductance quantization in quantum ballistic transport

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(Received 6 August 1990)

Using a generalized version of the gauge argument introduced by Laughlin in the discussion of the quantum Hall effect, the quantized conductance in a one-dimensional gas of charged fermions is related to the quotient of fermion charge and magnetic flux quantum, both in the presence and absence of a magnetic field. It is furthermore shown from the same arguments that, in the absence of a strong magnetic field, quantization is destroyed due to scattering. Finally, the crossover to the quantum Hall regime is discussed, employing the gauge argument.

I. INTRODUCTION

Following the experimental observation of conductance quantization in zero magnetic field^{1,2} a large number of theoretical papers³⁻⁵ have been published describing various ways of calculating quantum ballistic transport through constrictions. A question that has received relatively little attention, is whether the above-mentioned quantization and the quantum Hall effect have a common origin. This is an important issue, as a common origin of both effects would indicate that, *in principle*, some kind of fractional conductance quantization could also exist in one-dimensional (1D) structures due to electron correlation effects. In one of the first theoretical papers discussing the quantum Hall effect after its discovery,⁶ Laughlin⁷ explained the exactness of the quantization using a gauge argument. In the same paper the issue of the insensitivity of the quantization to scattering was addressed. Nowadays this is believed to be caused by the absence of backscattering in strong magnetic fields.⁸ Contrary to the situation in the quantum Hall effect, where scattering even widens the Hall plateaus, in the zero-field case, scattering is known to destroy quantization. This follows both from experimental data and from numerical work including scattering centers.^{4,5} In the first experimental paper a series resistance was subtracted from the experimental data in order to compensate for the effect of the current-voltage contacts. A disadvantage of this procedure is that it masks possible deviations of the quantized steps due to scattering close to the point contact. In other experiments either a four-terminal setup was used,² where one must somehow take care of the corrections due to the finite size of the wide regions in the four-terminal Landauer formula⁹ or a two-terminal setup with low-Ohmic contacts was used.¹⁰ Generally one observes a reduction of the conductance at the plateaus below the quantized values.¹¹ The best quantization observed to date is still of the order of a percent below the quantized values,¹⁰ while additional structure develops at the plateaus, especially at low temperatures and in the

presence of scattering.¹⁰⁻¹³

In order to demonstrate the common origin of both types of quantization, I generalize the construction used by Laughlin in the discussion of the quantum Hall effect to the case of the longitudinal resistance of a 1D strip either with or without magnetic field. First we have to realize that the point contacts that are used in the experiments on zero-field quantization are basically short 1D channels. Experimentally the channels have to be short in order to reduce the effect of scattering. The coupling between the wide 2D half planes and the 1D channel enters the theoretical description of the mesoscopic device as an extra complication, which is, however, not of fundamental importance for the concept of quantization. In fact, it has already been stressed by Landauer before the experimental observations were made¹⁴ that a smooth coupling between the wide and narrow regions results in the absence of scattering. It was shown by Glazman *et al.*,³ and later by Yacobi and Imry¹⁵ that for $R/\lambda \gg 1$ (where R is the radius of curvature of the constriction walls and λ is the Fermi wavelength) the structure behaves essentially as a 1D channel with a finite number of 1D subbands at the Fermi level. In the absence of scattering, each channel contributes^{16,17,14} $I = e^2 V n v_F$, where V is the applied voltage, e is the electronic charge, $n = (2\pi)^{-1} \partial k / \partial E$ is the 1D unidirectional density of states per unit of length, and $v_F = \hbar^{-1} \partial E / \partial k$ is the Fermi velocity. We see that in the Landauer description the conductance quantization results from a cancellation between density of states and group velocity. On the other hand, in the description of the quantum Hall effect, Laughlin derived that the quantized units of conductance are given by the quotient of elementary charge and magnetic flux quantum. In this paper I discuss the relation between these two descriptions.

II. GAUGE TRANSFORMATIONS

Let us first consider the conductance of a perfect 1D strip that is smoothly connected to randomizing baths

on both sides. Application of a voltage V between the left-hand side and the right-hand side results in a relative shift eV of the electrochemical potential of left- and right-going states. If we take out a finite section of such a strip, and consider the distribution of the electrons in momentum space, we find that it corresponds to the energetically most favorable state under the constraint of fixed total electronic momentum, which for a section of length L_y amounts to $L_y neV/\hbar k_F$. Another way to look at this is that it represents the equilibrium distribution seen from a co-moving frame with a velocity $e^2 V/2\hbar k_F$. Of course this is only a meaningful concept if no momentum of the electrons can be transferred to other degrees of freedom of the sample, such as the phonon bath. Theoretically such a situation can easily be envisaged; however, for the convenience of those who insist on the presence of inelastic scattering I add that our thought experiment is at least meaningful on a time scale shorter than the inelastic decay time of the electrons. We now bend the strip and merge both sides together *without changing the difference in occupation between left- and right-going states*. Using this procedure we avoid possible confusion about the meaning of an applied voltage in a loop. Experimentally an imbalance between the occupation of clockwise states (CWS's) and counter clockwise states (CCWS's) is obtained by applying a time-dependent magnetic flux through the loop. The Faraday effect then causes an acceleration of the electrons in one direction. Unlike the situation in a superconducting loop, where the current carrying state is stable after the change in enclosed flux has been completed, in a metallic ring this state decays due to inelastic scattering. In what follows I will assume that this inelastic decay is sufficiently slow on the time scale of our thought experiment. In analogy to the situation in the strip, the state of the electrons in the ring can be thought of as an equilibrium distribution under the constraint of fixed electronic angular momentum.

Due to periodic boundary conditions in the loop, the k vectors of the CWS's and CCWS's are now quantized in units of $2\pi/L_y$, where L_y is the circumference of the loop. In Fig. 1(a) the quantized states and the occupations are indicated for the current carrying state of a ring that has only one subband occupied. Obviously one can always choose the circumference of the ring such that there is a sufficiently large difference in occupation between CWS's and CCWS's no matter how small the difference in chemical potential is. In the plot a free-electron parabola is displayed, but in what follows this is of no relevance. We now calculate the current in the loop by using the thermodynamical equation

$$I = c \frac{\partial U}{\partial \phi}, \quad (1)$$

where U is the total energy, c is the light velocity, and ϕ is the magnetic flux enclosed by the loop. Similar to Laughlin's treatment of the quantum Hall effect we adiabatically increase ϕ . After the adiabatic addition of one magnetic flux quantum has been completed, the many-electron wave function is exactly mapped into itself. We

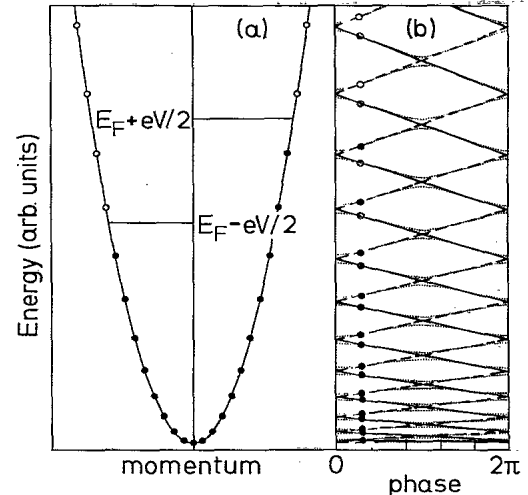


FIG. 1. (a) Energy dispersion of a perfect 1D closed loop. Due to the periodic boundary conditions k is quantized. Electrons occupying these quantized states are indicated for a situation where the loop encloses no magnetic flux. Also indicated is the difference in electrochemical potential between CCWS's and CWS's. (b) Reduced zone plot of the energy dispersion of (a) as a function of phase, i.e., $2\pi\phi/\phi_0$, where ϕ is the flux enclosed by the loop. Solid curves are clockwise states, dashed curves are counterclockwise states, and dotted curves are the opening of minigaps due to scattering.

furthermore observe that during the adiabatic change of ϕ the wave functions move along the single-electron dispersion curve of Fig. 1(a). This follows from the fact that the canonical momentum in the presence of an enclosed flux is given by $k + eA/(\hbar c)$, where A is the vector potential. As a result a phase factor $e^{2i\pi\phi/\phi_0}$ has to be added to the periodic boundary conditions, where ϕ_0 is the magnetic flux quantum (I use ϕ_0 to indicate h/e throughout this paper; in discussions of superconductivity Φ_0 is often used to indicate $h/2e$), so that the canonical momentum of the single-particle states transforms as

$$k \rightarrow k + 2\pi L_y^{-1} \frac{\phi}{\phi_0}.$$

Hence the net effect after increasing the enclosed flux with ϕ_0 is that one electron is transferred from a CWS at the Fermi level to a CCWS at the Fermi level. The corresponding increase in energy (ΔU) is eV ; hence the current is

$$I = c \frac{\delta U}{\delta \phi} = c(\phi_0)^{-1} eV. \quad (2)$$

Adopting the usual values of elementary charge and the elementary flux quantum, we arrive at the expression for the conductance

$$I/V = e^2/h. \quad (3)$$

Note that this shift register effect works only if each state is occupied by a single electron up to the Fermi level. One can check the importance of Fermi statistics at this point by trying to envisage what happens if the single-particle dispersion of Fig. 1 is subject to Bose statistics: The

ground state of such a system has all bosons in the lowest level. No applied voltage can exist, although a current flows if the bosons are condensed in a state with $k \neq 0$. This happens if the enclosed flux is a finite fraction of ϕ_0 . It is a manifestation of the fact that in a Bose condensate only diamagnetic currents can flow. From the above result we see that conductance quantization in units of e^2/h is a manifestation of the statistical properties of the electron gas. Due to the fact that a single electron is allowed in each (spin) state, precisely one electron is transferred in the adiabatic process. If electrons would obey another kind of statistics, e.g., if q electrons were allowed in each single-particle level up to the Fermi level, the unit of conductance quantization would be qe^2/h . One could regard spin degeneracy as a case where we have $q = 2$. However, in the presence of an external magnetic field, due to spin-orbit interactions, or due to exchange fields, the spin degeneracy is lifted. Hence, the two spin directions are usually treated as parallel quantum channels. In this context it is interesting to mention that fractional quantization of the conductance is accompanied by fractional statistics of the quasiparticle excitations.¹⁸ As the arguments used above are based on a single-particle picture of the ground state, these arguments can, however, not be directly applied to the many-body wave function describing the fractional quantum Hall state.

Equation (3) can easily be generalized to the quasi-1D case, where one has N nondegenerate occupied 1D subbands (not indicated in Fig. 1). The intersubband energy splitting plays the same role as the energy gap between Landau levels in the description of the quantum Hall effect.⁷ It prevents crossover between subbands in the adiabatic process. One has to add contributions of each subband to the total energy, resulting in

$$I/V = Ne^2/h. \quad (4)$$

III. SCATTERING

I now address the question of how scattering modifies the above result. In Fig. 1(b) the single-electron dispersion of Fig. 1(a) is displayed as a function of flux enclosed by the loop. For a fixed gauge the electrons occupy a discrete set of energy levels for each value of ϕ . The CWS's are indicated as solid curves, and the CCWS's are indicated as dashed curves. We see that each CWS crosses a CCWS at $\phi = \phi_0/2$. Hence, under adiabatic change of the enclosed flux the electrons can, in principle, move from a CWS to a CCWS at this point, provided that some scattering mixes these two bands. In fact, scattering results in the opening of minigaps,¹⁶ as indicated in Fig. 1(b). It is immediately clear that in the above-mentioned adiabatic process each electron returns to its original energy position. As a result the increase in energy ΔU is zero and there is no net current. Of course this is just a manifestation of 1D localization in the thermodynamic limit.¹⁹ This does not mean that for a wire of finite length the resistance is infinite. In fact, there exists an intimate

relation between the minigaps in a loop structure and the transmission coefficients in a linear structure, which I will describe in the following section. We see that our gauge argument leads to nonquantized conductances in the presence of scattering. This is equally true in the case of the quantum Hall effect, as I will briefly discuss in the last section. This result does not depend on the presence or absence of intersubband scattering (or inter-Landau-level scattering in the case of the quantum Hall effect), but rather on the presence of backscattering. Backscattering can be heavily suppressed in the presence of high magnetic fields, which causes the high precision of the resistance standard based on the quantum Hall effect. This high precision does not, however, follow from a gauge argument. The importance of the gauge argument is that it allows us to relate macroscopic transport properties to certain microscopic physical constants by employing the fact that electrons obey Fermi statistics.

IV. RELATION BETWEEN MINIGAPS AND TRANSMISSION

Scattering is introduced in a linear strip by including a portion of imperfect transmission, characterized by the scattering matrix S :

$$S = \begin{pmatrix} t & r \\ -r^* & t^* \end{pmatrix} e^{2i\mu}. \quad (5)$$

With this convention for the ordering of transmission coefficients t and reflection coefficients r , S is the unit matrix in the absence of scattering. In a different context quite often a notation is used, where r is the diagonal element.²⁰ The latter notation deserves preference when multiprobe configurations are considered. In a multiprobe problem the phrase "absence of scattering" no longer has an obvious physical meaning. In order to diagonalize S , the basis of left- and right-going states (LGS's and RGS's) has to be transformed to another two-dimensional basis, which depends on the properties of the disordered part of the strip. We reserve the indices $+$ and $-$ to indicate the basis vectors on which S is diagonal:

$$|k_+\rangle = \cos \theta e^{i\alpha} |k_{\text{RGS}}\rangle + \sin \theta |k_{\text{LGS}}\rangle, \quad (6)$$

$$|k_-\rangle = \sin \theta e^{i\alpha} |k_{\text{RGS}}\rangle - \cos \theta |k_{\text{LGS}}\rangle.$$

The parameters θ , α , and η_{\pm} are obtained by applying the orthogonal transformation, defined by Eq. (6), to the S matrix and by imposing diagonality:

$$\theta = \frac{1}{2} \arctan \left(\frac{|r|}{\text{Im}(t)} \right),$$

$$\alpha = \pi/2 - \arg(r), \quad (7)$$

$$\eta_{\pm} = \mu \pm \frac{1}{2} \cos^{-1} \text{Re}(t).$$

The diagonal matrix elements of S are $\exp(2i\eta_{\nu})$; η_{ν} is

called the scattering phase shift. The physical meaning of this is that a wave $|k_\nu\rangle$ incident to the scattering part is scattered into an outgoing wave $| - k_\nu\rangle$. During this process the wave acquires a phase shift, whereas the wave amplitude is conserved. The transmission and reflection coefficients are now readily obtained from an orthogonal transformation from the + and - basis to the RGS and LGS basis, resulting in

$$\begin{aligned} te^{2i\mu} &= \cos^2\theta e^{2i\eta_+} + \sin^2\theta e^{2i\eta_-}, \\ re^{2i\mu} &= \sin\theta \cos\theta e^{-i\alpha} (e^{2i\eta_+} - e^{2i\eta_-}). \end{aligned} \quad (8)$$

The parameters θ and α are determined by the scattering potential. In principle, they also depend on external parameters such as electron density and magnetic field. The same holds true for the scattering phase shifts. In many physical situations, however, the phase shifts have a much stronger dependence on external parameters. For example, if the electron density is such that the Fermi energy lies close to a resonance, the change in phase shift in moving the Fermi level through the resonance is π , whereas θ and α are, in principle, unaffected by the resonant behavior. This is also known as Levinson's theorem. In a number of cases one can easily see that θ is a constant. For example, if there is time-inversion symmetry, we have $t = t^*$, and hence, using Eq. (7), $\cos^2\theta = \frac{1}{2}$. In the case of inversion symmetry (i.e., point inversion symmetry if there is no time-reversal symmetry; otherwise a mirror plane perpendicular to the current direction suffices), the basis is formed by even and odd subbands along y , and again $\cos^2\theta = \frac{1}{2}$.²¹ The phase shifts have to be calculated from the perturbation Hamiltonian of the scattering part. The connection can be made by applying the optical theorem

$$S = 1 + 2i(\text{Im}g)T.$$

This is an exact identity, which in this form relates the scattering matrix in diagonal form to the Green's function g of the unperturbed system and the transition matrix T , which is the dressed perturbation Hamiltonian containing all vertex corrections. From comparison with the S -matrix elements in diagonal form we immediately obtain

$$\eta_\nu = \arg(T_{k\nu}^{k\nu}). \quad (9)$$

From the transition-matrix Dyson equation

$$T = H^1 + H^1GH^1,$$

where H^1 is the perturbation matrix and G is the Green's function of the perturbed system, we can calculate the matrix elements of T :

$$\begin{aligned} \text{Re}T_{k\nu}^{k\nu} &= \langle k\nu|H^1|k\nu\rangle + \langle k\nu|H^1(\text{Re}G_\nu)H^1|k\nu\rangle, \\ \text{Im}T_{k\nu}^{k\nu} &= \langle k\nu|H^1(\text{Im}G_\nu)H^1|k\nu\rangle. \end{aligned} \quad (10)$$

We now define

$$\begin{aligned} V_\nu &\equiv \text{Re}T_{k\nu}^{k\nu}, \\ \rho_\nu^* &\equiv \pi^{-1}V_\nu^{-2}\text{Im}T_{k\nu}^{k\nu}. \end{aligned} \quad (11)$$

With these definitions we now see that the phase shifts are

$$\eta_\nu = \arctan(V_\nu\rho_\nu^*).$$

In lowest-order perturbation theory ρ_ν^* is the unidirectional density of states $L_y/(hv_F)$. For larger values of the perturbation Hamiltonian H^1 , ρ_+^* , and ρ_-^* reflect a "dressed" or "effective" density of states. We are now able to work out an explicit expression for the transmission coefficient:

$$|t|^2 = \frac{\sin^2(2\theta)}{1 + [\pi(V_+\rho_+^* - V_-\rho_-^*)/(1 + \pi^2V_+V_-\rho_+^*\rho_-^*)]^2 + \cos^2(2\theta)}. \quad (12)$$

Note that the term V_+V_- in the denominator effectively acts as a higher-order correction to the term $(V_+\rho_+^* - V_-\rho_-^*)$. Here we come to the central step, allowing us to make the connection between transmission coefficients and gaps: If we now take the strip and again bend it to form a loop structure, the minigaps at the points where $|k_{\text{CWS}}\rangle$ and $|k_{\text{CCWS}}\rangle$ cross are in lowest-order perturbation theory given by

$$\begin{aligned} E_g &= \langle k_+|H^1|k_+\rangle - \langle k_-|H^1|k_-\rangle \\ &= (V_+ - V_-) + O((H^1)^2). \end{aligned} \quad (13)$$

That is, in this order of perturbation theory V_+ and V_- represent the upward and the downward shift of the eigenstates, which are formed by mixing $|k_{\text{CWS}}\rangle$ and $|k_{\text{CCWS}}\rangle$. We can make the identification more explicit by defining an effective ρ^* and E_g^* :

$$\begin{aligned} \rho^* &\equiv \sqrt{\rho_+^*\rho_-^*}, \\ E_g^* &\equiv \frac{V_+\sqrt{\rho_+^*/\rho_-^*} - V_-\sqrt{\rho_-^*/\rho_+^*}}{1 + \pi^2V_+V_-\rho_+^*\rho_-^*}. \end{aligned} \quad (14)$$

Using these definitions we finally arrive at the following expression relating the conductance of a 1D strip to the minigaps in an equivalent ring structure:

$$|t|^2 = \frac{\sin^2(2\theta)}{1 + (E_g^*\pi\rho^*)^2} + \cos^2(2\theta). \quad (15)$$

If there is either time-reversal symmetry or inversion symmetry the formula has a simpler form, as in the case we have of $\sin^2(2\theta) = 1$:

$$\frac{h}{e^2} \frac{I}{V} = \frac{1}{1 + (E_g^*\pi\rho^*)^2}. \quad (16)$$

In the absence of a magnetic field, the size of the mini-

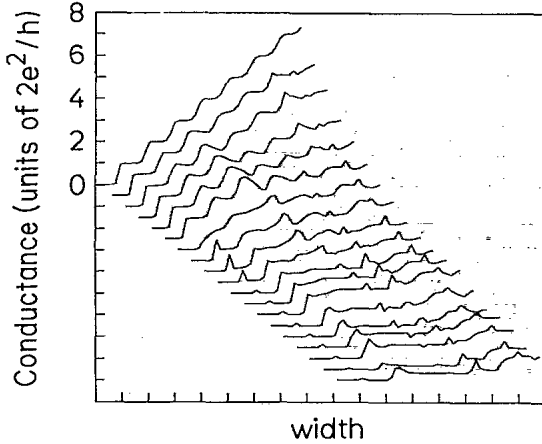


FIG. 2. Conductance vs constriction width for a constriction with a varying amount of disorder. The size of the area was 1.6 Fermi wavelengths in the current direction and 4.0 Fermi wavelengths perpendicular to this. The length of the constriction was kept at 0.5 Fermi wavelengths, and the width is the parameter varied along the horizontal axis and is swept from 0 to 4.0 Fermi wavelengths. The number of impurities added is between 0 and 90 with increments of 5 from top left to bottom right. For clarity the curves have been given diagonal offsets at regular intervals.

gaps is proportional to the density of scattering centers. Hence, for each channel $1 - |t|^{-2}$ is proportional to n^2 , where n is the 2D impurity density. In Fig. 2 this is further illustrated by the results of a numerical simulation of the effect of adding impurities to a constriction between two infinite 2D half planes, using the formalism outlined in Ref. 5. In the simulation δ -function impurities were added at random to a rectangular region adjacent to the constriction area. We see from the values of the conductance at the plateaus that the conducting channels roughly follow the expected behavior, each with a different prefactor, i.e., the size of each step decreases roughly proportional to n^2 and asymptotically approaches zero. The details of the suppression of the conductance at each plateau depend strongly, of course, on the precise location of the impurities. A single δ -function impurity has the effect of completely suppressing the wave amplitude in a region of about a quarter of a wavelength.⁵ The matrix elements V_i are therefore proportional to the kinetic energy times the Fermi wavelength divided by the length of the loop. Hence $E_g \simeq 0.5E_F\lambda_F/L_y$. The reduction of the transmission due to a δ -function impurity placed inside the constriction is then approximately 15%, which agrees with the numerical results of Ref. 5. There are additional effects, which become stronger as the disorder increases, such as the formation of virtual bound states, which gives rise to resonance peaks at certain values of $k_F W$. I have to add here that the numerical calculations are exact and hence also incorporate intersubband scattering, an effect that is not included in our simple 1D formula Eq. (15).

V. MAGNETIC FIELDS

In the presence of a strong magnetic field this situation changes drastically. Let us first assume that there is no scattering. Again the same gauge arguments can be used.⁷ On increasing the magnetic-field strength the dispersion relation of Fig. 1 gradually develops into a dispersionless band for $|k| \ll L_x/(2l_B^2)$, with a steep rise for k close to $\pm L_x/(2l_B^2)$, where L_x is the width of the strip and $l_B = (\hbar c/|eB|)^{1/2}$ is the magnetic length. An important difference is that the wave functions with different k vectors become spatially separated along the direction perpendicular to the current path, i.e., the guiding centers are given by the following expression:

$$\begin{aligned} y_0 &= \left[-k + \left(\frac{\phi}{\phi_0} \right) \left(\frac{2\pi}{L_y} \right) \right] l_B^2 \\ &= -kl_B^2 + \left(\frac{\phi}{\phi_0} \right) \left(\frac{L_x(i)}{N(i)} \right), \end{aligned} \quad (17)$$

where $N(i)$ is the number of k states in the flat portion of the i th subband, and $L_x(i)$ is the corresponding effective sample width. As a result, the spatial separation between crossing CWS's and CCWS's close to the integer filling factor of a Landau level is of the order of the sample width L_x ; i.e., they correspond to opposite edge channels.²² If we now introduce scattering, in principle minigaps will open, as in the case where we had zero applied field. The occurrence of minigaps in this case has been treated by Aoki.²³ The matrix elements determining the minigaps are then proportional to $\exp[-(L_x/4l_B)^2]$.²⁴ If we insert this in Eq. (15) we obtain an exponentially small correction on the conductance.

VI. CONCLUSIONS

From a gauge argument it is shown that the occurrence of e^2/h reflects the (Fermi) statistical properties of the electron gas, both for the quantum Hall effect and for the much less robust conductance quantization in a point contact. In principle, in both regimes the conductances are reduced from the exact quantized values. However, in the limit of high magnetic fields ($L_x/l_B \gg 1$) the exponentially small parameter $\exp[-(L_x/4l_B)^2]$ determines the corrections to the quantized conductance in the presence of scattering, whereas in the low-field regime ($L_x/l_B \ll 1$) scattering has a pronounced influence on the quantized conductance.

ACKNOWLEDGMENTS

The author is grateful to Professor Dr. K. von Klitzing and J. Nieder for stimulating discussions during preparation of this document, and to Dr. A. D. Wieck, Dr. C. W. J. Beenakker, and Professor Dr. R. Gerhardt for useful comments on the manuscript.

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