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Leaky and mutually coupled quantum wires

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In this paper, we investigate the effect on the transport in a quantum wire of short-ranged irregularities in the boundary. The results obtained are generalized to the case of a small hole in the boundary. Via such a hole, the wire is coupled to free two-dimensional space or to a second wire. Some interesting resonance features in the transmissivities are found and it is shown that the flux through the orifice exhibits narrow peaks at energies where quasibound states in one of the wires are possible. These fluxes are on the order of the currents inside the wire and thus should be measurable by experiment. We use a multiple-scattering formalism in terms of renormalized scattering amplitudes. This method turns out to be well suited for this kind of problem because it allows a very compact formulation, as has been shown in previous papers.

I. INTRODUCTION

Some years ago, advanced fabrication techniques made it possible to produce microstructures which are called quantum wires. If the mean free path is large compared to the system dimensions, electrons can move ballistically through the wire. For such ballistic wires, the conductance was found to be quantized in steps of e^2/h.[1,2] Soon after the theoretical clarification of the quantized conductance, attention was paid to the influence of perturbations in ballistic wave guides on the conductance.[3]

In order to calculate the conductivity, the transmission matrices t are calculated and then related to the conductivity using the Landauer-Büttiker formula, $G \sim t^+ t$.[4]

Many papers have addressed the scattering problem of impurities inside the wire. Single impurities[5–11] as well as scatterer ensembles[12,13] and wires that are filled uniformly with scatterers[14,15] have been considered. The main result of all these papers is that the presence of impurities in the wire decreases the conductivity from its ballistic value and gives rise, in certain cases, to huge fluctuations of the transmissivity.[13] Other interesting results are that resonances at single impurities can cause transparency or quasibound states (QBS) (Refs. 5, 7, 10, and 11) which cause sharp downward dips in the conductance plot. While most of the models for quantum wires assume rectilinear wave guides, short-range impurities in wires with more realistic confinement potentials were investigated, too.[6] These theoretical findings were confirmed, at least qualitatively, by experiments.[16–18]

Another focus is the role of surface irregularities in quantum transport systems. The action of small bumps or holes on edge states under magnetic fields was considered,[19] as well as resonant transport through openings that are small compared to the electron wavelength,[20] and surface roughness.[21] Another paper[22] investigates the action of boundary corrugations of a quantum wire in the context of localization theory. It is restricted to the first subband and shows that volume and surface scattering have qualitatively the same action on the transport in quantum wires.

The method that is most often used for the mathematical description of short-ranged surface perturbations is the so-called Kirchhoff integral method.[23–25] In Ref. 19, the scattering amplitudes for various kinds of surface irregularities are obtained by means of conformal mapping. Here we will use some of these results.

Recent work is dedicated to a variety of coupled quantum systems. Among them, the connection of a quantum wire to a side branch via a tunnel barrier in the context of quantum point spectroscopy can be found,[26] a possible switch device of two coupled wires[27] or a resonator attached to a wire.[28,29] Considerable interest was directed to crossed quantum wires, in particular to the bound states in the cross region.[30–32]

Our paper contributes to the problem of a quantum wire coupled either to infinite space or to another wire via a small hole. We obtain analytic expressions for the transmissivity along the wire, from the wire to free space, or between two wires for the limiting cases where either the connection is much longer than its width or vice versa. The first limit models a probe attached to the wire which ensures a very weak coupling of outer and inner regions. The other limit gives rise to considerable fluxes through the hole at energies at which QBS in the wire become possible.

The scattering formalism we employ is based on the concept of so-called renormalized scattering amplitudes, $\tilde{f}$.[14,7] An equivalent formulation using a slightly different language can be found in Refs. 6, 33, and 34. The idea is that the field incident on a scatterer in a wire comprises not only the primary wave but also an additional contribution due to repeated backscattering processes between the scatterer and the confinement. All these contributions are summed up and are represented by a quantity called the backscattering amplitude. The renormalized scattering amplitude enables us to work with the primary field (instead of the actually incident field) when considering the scattering process. Another ingredient of our method is the local density of states (LDOS). It holds a

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central role in the whole formalism. The scattering amplitude is related to the LDOS by the optical theorem which helps to simplify some expression. For example, QBS appear very naturally as poles of $\tilde{f}$. In order to obtain their energy and decay width it is sufficient to consider only the backscattering amplitude and LDOS.

This method has been used in the compact formulation of the "short-ranged scatterer in a wire" problem, without[7,6] and with magnetic fields,[8,9] and in the investigation of bound states in crossed magnetic and electric fields.[33] It turned out to be well-suited for these problems and therefore we apply it now to the problem of surface irregularities in a wire. In this sense, the present paper is a direct continuation of our previous work.[7] It provides a good insight into the physics behind and gives general information beyond numerical results.

The only restriction to the irregularities is that they are of short-ranged type, i.e., the electron wavelength is large compared to the characteristic dimensions of the surface perturbation. It is modeled in two dimensions, according to two-dimensional confined electron gases (2DEG). Thus our model is comparable to others.[19,20,28,29] The wire is laterally confined by hard boundaries.

Our paper is organized as follows: In Sec. II, the elementary two-dimensional (2D) scattering problem of a surface irregularity is formulated and solved and the optical theorem for such a scatterer is derived. Furthermore, the generalized formulas are given if the perturbation is of open type. Section III is dedicated to the scattering problem of an irregularity in the confinement of a wire for closed bumps and for openings. The transmissivities along the wire and out of the wire are obtained analytically. In Sec. IV, the transport problem for two quantum wires coupled by a small orifice is considered and the transmission coefficients are derived. The dependence of the transmissivities found in Secs. III and IV on energy is analyzed in Sec. V. Special attention is paid to the QBS because their presence gives rise to sharp resonances of the transmission coefficients. Finally, Sec. VI gives conclusions and main results.

II. THE SCATTERING PROBLEM OF A 2D BOUNDARY IRREGULARITY

In the first step we consider the 2D scattering problem of a hard straight boundary with a bump, see Fig. 1(a). The linear dimensions a of the perturbation are assumed to be small compared to the electron wavelength, i.e., $a \ll \lambda$.

The wave equation is, as usual,

$$\left[\frac{\partial^2}{\partial \mathbf{r}^2}+k^2\right]\Psi(\mathbf{r})=0, \quad \mathbf{r}=(x,y) , \tag{1}$$

with the boundary condition that $\Psi(\mathbf{r})$ vanishes along the boundary. The wave number k is related to the particle energy E by $E=(\hbar^2/2m)k^2$.

The Green's function for a 2D half-space with a straight boundary at $y=0$ is the sum of two propagators of the empty 2D space, according to direct propagation and specular reflection at the boundary,

$$G_0(\mathbf{r},\mathbf{r}')=\frac{i}{4}\left\{H_0^{(1)}\left[k\sqrt{(x-x')^2+(y-y')^2}\right] - H_0^{(1)}\left[k\sqrt{(x-x')^2+(y+y')^2}\right]\right\} , \tag{2}$$

where $H_0^{(1)}$ is Hankel's function of the first kind and zeroth order.[35,25] G_0 satisfies the differential equation

$$\left[\frac{\partial^2}{\partial \mathbf{r}^2}+k^2\right]G_0(\mathbf{r},\mathbf{r}')=-\delta(\mathbf{r},\mathbf{r}') . \tag{3}$$

Let $\phi_0(\mathbf{r})$ be a primary field that obeys the boundary condition for a straight, unperturbed boundary. Then, if the boundary contains a short-ranged irregularity located around $\mathbf{r}_0=(x_0,0)$ with a height profile $h(x)$, the wave function is the superposition of primary and scattered field,

$$\Psi(\mathbf{r})=\phi_0(\mathbf{r})+\Psi_{sc}(\mathbf{r}) . \tag{4}$$

Ψ_{sc} can be obtained using the Kirchhoff integral method[19,20,22,23,25,35]

$$\Psi_{sc}(\mathbf{r})=k\int_{\text{boundary}}[G_0(\mathbf{r},\mathbf{r}')\partial_n'\Psi(\mathbf{r}') - \Psi(\mathbf{r}')\partial_n' G_0(\mathbf{r},\mathbf{r}')]ds' , \tag{5}$$

where the integration is performed over the boundary

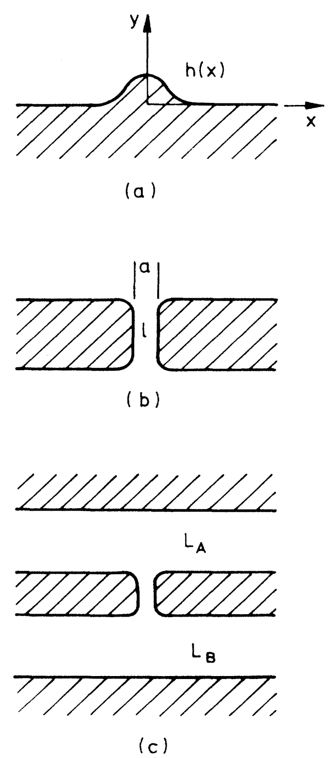

FIG. 1. The model boundary irregularities. (a) Bump on a boundary with a height profile $h(x)$. The characteristic dimensions of the irregularity are of order a. (b) Orifice with width a in a hard wall of thickness l. (c) Two parallel quantum wires connected by an orifice.

containing the irregularity. We have defined the operation $\partial_n \equiv \partial / k \partial \mathbf{n}$ as the (inward) normal derivative taken on the boundary. The derivatives are normalized to k for later convenience. Since $\Psi=0$ holds everywhere on the boundary, the second term in (5) vanishes. In addition, since $G_0=0$ holds along the unperturbed boundary, contributions to the integral come from the distorted region only:

$$\Psi_{sc}(\mathbf{r})=k\int_{\rm bump} G_0(\mathbf{r},\mathbf{r}')\partial_n'\Psi(\mathbf{r}')ds' \ . \tag{6}$$

In particular, as follows from (6), for the incident field we obtain

$$\partial_n\Psi(\mathbf{r})=\partial_n\phi_0(\mathbf{r})+k\int_{\rm bump}\partial_n G_0(\mathbf{r},\mathbf{r}')\partial_n'\Psi(\mathbf{r}')ds' \ . \tag{7}$$

For a sufficiently smooth perturbation profile we can approximate the incident field by $\partial_n\Psi(\mathbf{r})\approx\partial_n\phi_0(\mathbf{r}) =\partial_0\phi_0(\mathbf{r})\cos\varphi_n$ where φ_n is the angle between the normals of the perturbation and the unperturbed boundary, respectively, and $\partial_0'\equiv(\partial/k\partial y')_{\mathbf{r}_0}$ has been defined for the sake of brevity. Because of the smallness of the bump, G_0 can be expanded with respect to $\mathbf{r}_0$. Now we have for (6)

$$\begin{aligned}\Psi_{sc}(\mathbf{r})&\approx-\left[\frac{\partial}{k\partial y''}\right]_{\mathbf{r}_0}\phi_0(\mathbf{r}'')\left[\frac{\partial}{k\partial y'}\right]_{\mathbf{r}_0}G_0(\mathbf{r},\mathbf{r}')\\ &\qquad\times\int_{\rm bump}k^2h(x')\cos\varphi_{n'}ds'\\ &\approx\partial_0''\phi_0(\mathbf{r}'')\partial_0'G_0(\mathbf{r},\mathbf{r}')f \ .\end{aligned} \tag{8}$$

The derivatives of ϕ_0 and G_0 are constants within the bump region, and the remaining integral gives approximately the scattering amplitude f of the short-ranged bump. Note that f is still purely real in this approximation because we have used only the near-field asymptotics of ϕ_0 and G_0 and thus the wave nature has been suppressed. The (much smaller) imaginary part of f will be calculated below.

From (8) we see that scattering at short-ranged irregularities on hard walls is described by the normal derivative of the incoming field and that of the Green's function, mediated by a scattering amplitude f. The order of f can be evaluated from the integral in (8) to be $f\sim(ka)^2$ for convex bumps [i.e., $h(x)<0$], and $f\sim-(ka)^2$ for concave ones [$h(x)>0$], cf. also Ref. 19. (Note the difference from usual 2D s scatterers where $f\sim\ln ka$.[6,33])

For any scattering amplitude f one can derive a relation that is called optical theorem. It ensures that the current density of the total field (4) is source-free at $\mathbf{r}_0$ and relates the imaginary part of a scattering amplitude to the local density of states and to $|f|^2$. Here, we use it in order to get Imf from $|f|^2\approx$ Ref which we have obtained in (8). At first glance, Imf could seem to be negligible due to its smallness. But it plays an important role in backscattering resonances. Discussions of resonance phenomena at s scatterers where the optical theorem holds a central position are provided in Refs. 7–9. Here, we derive it for the special case of short ranged surface scatterers.

The current density of the electron wave is

$$\mathbf{j}(\mathbf{r})=\mathrm{Im}\left[\Psi^*(\mathbf{r})\frac{\partial}{\partial\mathbf{r}}\Psi(\mathbf{r})\right] \tag{9}$$

and thus

$$\frac{\partial}{\partial\mathbf{r}}\mathbf{j}(\mathbf{r})=\mathrm{Im}\left[\Psi^*(\mathbf{r})\frac{\partial^2}{\partial\mathbf{r}^2}\Psi(\mathbf{r})\right] \ . \tag{10}$$

Expression (10) must be zero everywhere for a source-free current. Inserting (4) into (10) and using the second line of (8) for Ψ_{sc} we get

$$\mathrm{Im}[(\phi_0^*(\mathbf{r})+\partial_0'(\mathbf{r}')\partial_0'G_0^*(\mathbf{r},\mathbf{r}')f^*)\partial_0'\phi_0(\mathbf{r}')f]\partial_0'\delta(\mathbf{r},\mathbf{r}')=0 \ . \tag{11}$$

We remark that the derivative of the δ function is rather a formal expression without mathematical rigidity and follows from the derivative of the Green's function in (8). Nevertheless, if we perform the limit $\mathbf{r}\to\mathbf{r}_0$ it yields

$$\mathrm{Im}f=|f|^2\partial_0\partial_0'\mathrm{Im}G_0(\mathbf{r},\mathbf{r}')\equiv|f|^2\hat{A}\ \mathrm{Im}G_0 \ . \tag{12}$$

This is the required optical theorem for short-ranged surface scatterers. It looks very similar to that of isolated scatterers; see Ref. 36. So, $\hat{A}$ ImG_0 plays here the role of the LDOS. With the Green's function (2) we find $\hat{A}$ Im$G_0=\frac{1}{4}$ which does not depend on energy for the 2D case. The left-hand side of (12) originates from the interference of an incoming field and a scattered wave, whereas the term on the right-hand side is proportional to the current emerging from a point source with effectivity $|f|^2$ located in the boundary.

If the irregularity is of an open type, see Fig. 1(b), we define two different scattering amplitudes: f^+ for scattering back into the region where the incident field comes from, i.e., $y>0$, and f^- for scattering into the region "behind" the wall, i.e., $y<-l$, where l is the thickness of the wall. Hence, there are two expressions for the wave function:

$$\Psi(\mathbf{r})=\phi_0(\mathbf{r})+\partial_{0+}'\phi_0(\mathbf{r}')f^+\partial_{0+}''G_{0+}(\mathbf{r},\mathbf{r}'') \ , \quad y>0 \ , \tag{13}$$

and

$$\Psi(\mathbf{r})=\partial_{0-}'\phi_0(\mathbf{r}')f^-\partial_{0-}''G_{0-}(\mathbf{r},\mathbf{r}'') \ , \quad y<-l \ , \tag{14}$$

where ∂_{0+} has to be taken at $\mathbf{r}_0$ whereas ∂_{0-} is the normal derivative on the "backside" of the orifice, i.e., at $\mathbf{r}_0-l\hat{e}_y$. Accordingly, $G_{0+}(\mathbf{r},\mathbf{r}')$ is the Green's function for the half-space $y>0$ and $G_{0-}(\mathbf{r},\mathbf{r}')$ is that for $y<-l$.

In Ref. 19, the quantities $|f^+|^2$ and $|f^-|^2$ have been calculated by means of a conformal mapping technique for the limit of a long orifice, $l\gg a$ as well as for the opposite case, $l\ll a$. Here, we cite these results without derivation:

$$\begin{aligned}&a\ll l\colon\ |f^-|^2\sim\exp\left[-\frac{l}{\pi a}\right] \ , \ |f^+|^2\sim(ka)^4 \ ,\\ &a\gg l\colon\ |f^-|^2\sim|f^+|^2\sim(ka)^4 \ .\end{aligned} \tag{15}$$

For the case of an open perturbation, the sign of f^- must be negative according to our considerations after Eq. (8). In the limit of an infinitely thin wall, the equality

$|f^-|^2=|f^+|^2$ holds.

In the present paper, the ratio $|f^-/f^+|^2$ will hold a central role. In general, it seems to be difficult to compute it exactly from a given orifice geometry. For our considerations, however, it should be sufficient to assume it to be in the order of unity for short holes. As one can expect, only these orifices guarantee a considerable coupling.

Finally, we show how the optical theorem (12) is altered in the case of an orifice. On the right-hand side of Eq. (12) there occurs now an additional term which originates from the current into the region $y<-l$. The left-hand side remains unchanged because the incoming wave and the wave at $y<-l$ do not interfere. Thus the generalized optical theorem reads as

$$\mathrm{Im} f^+=|f^+|^2\hat{A}_+\mathrm{Im}G_{0+}+|f^-|^2\hat{A}_-\mathrm{Im}G_{0-}\ , \tag{16}$$

where again the subscripts denote the side where the derivatives have to be taken.

III. THE SCATTERING PROBLEM OF A BOUNDARY IRREGULARITY IN A SINGLE WIRE

Now we consider a rectilinear ballistic wire confined by two hard walls at $y=0$ and $y=L$, respectively. At $r_0=(0,0)$ the boundary contains either a bump or an orifice that connects the wire to free 2D space. Such an opening can serve as a model for probes attached to the wire.

The (normalized) wave function of the unperturbed wave guide in mode n is

$$\phi_{0,n}(\mathbf{r})=\left[\frac{2}{L}\right]^{1/2}\sin n\kappa y\ \exp ik_n x \tag{17}$$

with $\kappa=\pi/L$ and $k_n=\sqrt{k^2-n^2\kappa^2}$, and the Green's function inside the wire is

$$G_{\mathrm{wire}}(\mathbf{r},\mathbf{r}')=\sum_n \frac{i}{L\kappa_n}\sin n\kappa y\ \sin n\kappa y'\exp ik_n|x-x'|\ . \tag{18}$$

The scattering problem of the boundary perturbation is treated in analogy to the preceding section: the derivatives of the incident field and the Green's function, respectively, are the quantities that describe the scattering process.[22] However, the field actually incident on the perturbation is not only the primarily incoming field but includes also a part which results from multiple backscattering between the bump and the walls.

Let the primary wave be $\phi_{0,n}$. The total wave field inside the wire is now

$$\Psi_{\mathrm{wire}}(\mathbf{r})=\phi_{0,n}(\mathbf{r})+\partial'_{0+}\phi_{\mathrm{inc},n}(\mathbf{r}')f^+\partial''_{0+}G_{\mathrm{wire}}(\mathbf{r},\mathbf{r}'') \tag{19}$$

and outside, if the perturbation is an orifice,

$$\Psi_{\mathrm{out}}(\mathbf{r})=\partial'_{0+}\phi_{\mathrm{inc},n}(\mathbf{r}')f^-\partial''_{0-}G_{0-}(\mathbf{r},\mathbf{r}'')\ . \tag{20}$$

∂_{0+} and ∂_{0-}, respectively, are defined as in the preceding section as normal derivatives taken at $y=0$ and $y=-l$, respectively. According to our above considerations, $\partial_{0+}\phi_{\mathrm{inc},n}(\mathbf{r})$ is the derivative of the actually incident field and can be written as the sum of primary wave and the part resulting from backscattering:

$$\partial_{0+}\phi_{\mathrm{inc},n}(\mathbf{r})=\partial_{0+}\phi_{0,n}(\mathbf{r})+\partial_{0+}\phi_{\mathrm{inc},n}(\mathbf{r})f^+G_b\ . \tag{21}$$

G_b is called backscattering amplitude. It can be thought of as a wave starting at the perturbation and being reflected *at least once* at one of the boundaries. This wave corresponds to a quantity $\partial'_{0+}[G_{\mathrm{wire}}(\mathbf{r},\mathbf{r}')-G_{0+}(\mathbf{r},\mathbf{r}')]$, cf. Ref 7. Finally, this wave acts as an incident field on the perturbation which yields a derivative again. Thus we get

$$\begin{aligned} G_b&=\partial_{0+}\partial'_{0+}[G_{\mathrm{wire}}(\mathbf{r},\mathbf{r}')-G_{0+}(\mathbf{r},\mathbf{r}')]\\ &=\hat{A}_+[G_{\mathrm{wire}}-G_{0+}] \end{aligned} \tag{22}$$

with $\hat{A}_+$ as defined in Eq. (16).

With (21) we can write Eq. (19) more compactly as

$$\Psi_{\mathrm{wire}}(\mathbf{r})=\phi_{n,0}(\mathbf{r})+\partial'_{0+}\phi_{0,n}(\mathbf{r}')\tilde{f}^+\partial''_{0+}G_{\mathrm{wire}}(\mathbf{r},\mathbf{r}'') \tag{23}$$

with the "renormalized scattering amplitude"

$$\tilde{f}^+=f^+\frac{1}{1-f^+G_b}\ . \tag{24}$$

In the same way, Eq. (20) can be written as

$$\Psi_{\mathrm{out}}(\mathbf{r})=\partial'_{0+}\phi_{0,n}(\mathbf{r}')\tilde{f}^-\partial''_{0-}G_{0-}(\mathbf{r},\mathbf{r}'') \tag{25}$$

with

$$\tilde{f}^-=f^-\frac{1}{1-f^+G_b}\ . \tag{26}$$

It is clear that merely f^+ occurs in the renormalization factor because only this quantity is relevant for backscattering in the wire.

We can insert G_b from Eq. (22) into the denominator of the renormalized scattering amplitudes and use the optical theorem (16). Now $\tilde{f}^+$ and $\tilde{f}^-$ read as

$$\tilde{f}^+=\frac{1}{\mathrm{Re}\left[\frac{1}{f^+}-G_b\right]+i\left[\hat{A}_+\mathrm{Im}G_{\mathrm{wire}}+|f^-/f^+|^2\hat{A}_-\mathrm{Im}G_{0-}\right]},\quad \tilde{f}^-=\frac{f^-}{f^+}\tilde{f}^+\ . \tag{27}$$

From Eq. (27) we get the very satisfying result that for $\tilde{f}^+$ an optical theorem exists similar to Eq. (16):

$$\mathrm{Im}\tilde{f}^+=|\tilde{f}^+|^2\hat{A}_+\mathrm{Im}G_{\mathrm{wire}}+|\tilde{f}^-|^2\hat{A}_-\mathrm{Im}G_{0-}\ . \tag{28}$$

From the channel representation of the Green's function in a wire, Eq. (18), it follows that

$$\hat{A}_+\mathrm{Im}G_{\mathrm{wire}}=\sum_n^N\frac{n^2\kappa^2}{Lk_nk^2}\ . \tag{29}$$

N is the number of propagating modes. Well apart from mode thresholds, $\hat{A}_+\mathrm{Im}G_{\mathrm{wire}}$ is in the order of unity, but if the energy approaches a threshold from above it shows the typical divergences of the quasi-one-dimensional LDOS.

Now we will derive the transmissivities T_{wire} for the transport inside the wire as well as T_{out} for the flux out of the wire to the free 2D space through the small hole. They are obtained from the matrix t_{nm} via $T=t^+t$. It relates the amplitude of a primarily incoming wave in mode n to that of a transmitted wave in any mode m and guarantees flux conservation. With $\tilde{f}^+$ and $\tilde{f}^-$ we can write down t_{nm} in a very compact form, see Ref. 7. From Eq. (23) we get with the incoming wave $\phi_{0,n}$ in (17) and the channel representation (18) of the Green's function

$$t_{nm}=\delta_{nm}+i\tilde{f}^+\frac{nm\kappa^2}{L\sqrt{k_m k_n}k^2}\ . \tag{30}$$

Consequently,

$$\begin{aligned}T_{\mathrm{wire}}&=N-2\,\mathrm{Im}\tilde{f}^+\sum_n^N\frac{n^2\kappa^2}{Lk_nk^2}+|\tilde{f}^+|^2\left[\sum_m^N\frac{m^2\kappa^2}{Lk_mk^2}\right]^2\\&=N-|\tilde{f}^+|^2(\hat{A}_+\mathrm{Im}G_{\mathrm{wire}})^2\\&\quad-2|\tilde{f}^-|^2\hat{A}_+\mathrm{Im}G_{\mathrm{wire}}\hat{A}_-\mathrm{Im}G_{0-}\ .\end{aligned} \tag{31}$$

For the second equality in Eq. (31) we have used Eq. (29) and the optical theorem (28).

The terms that decrease the transmissivity T_{wire} from its ballistic value ($T_{\mathrm{wire}}=N$) correspond to rather simple expressions for fluxes that are either reflected in the wire or transmitted out of it. These fluxes are made up by the partial LDOS of incoming and outgoing states, respectively, mediated by the absolute square of the scattering amplitude for the related scattering process.[8,9] So, the term in (31) with $|\tilde{f}^+|^2$ corresponds to the current reflected in the wire, and it is obvious that for the part transmitted out of the wire remains

$$T_{\mathrm{out}}=2|\tilde{f}^-|^2\hat{A}_-\mathrm{Im}G_{0-}\,\hat{A}_+\mathrm{Im}G_{\mathrm{wire}}\ . \tag{32}$$

In Sec. V we will consider how T_{wire} and T_{out} depend on energy.

IV. TWO QUANTUM WIRES COUPLED BY A SMALL OPENING

Imagine now two quantum wires [see Fig. 1(c)], labeled A and B, coupled by a small hole. Wire A is confined at $y=0$ and $y=L_A$, whereas the boundaries of wire B are located at $y=-l$ and $y=-(l+L_B)$.

If we want to describe scattering within each wire as well as between them in a compact form similar to that in (23) and (25), we employ again the concept of renormalized scattering amplitudes and define $\tilde{f}^{AA}$ and $\tilde{f}^{BB}$ for scattering within each wire A or B. On the other hand, for scattering from wire A to wire B we define $\tilde{f}^{AB}$, and $\tilde{f}^{BA}$ for the opposite direction.

In this case, there is a complex interplay between backscattering effects on both sides and intermediate transmission through the coupler. Therefore, the renormalized scattering amplitudes must contain the backscattering amplitudes G_b^A and G_b^B of both wires as well as f^+ and f^-. G_b^A describes all backscattering cycles in wire A only and does not contain information about wire B. Consequently it is defined as

$$G_b^A\equiv\hat{A}_+[G_{\mathrm{wire}\,A}-G_{0+}]\ . \tag{33}$$

Accordingly, G_b^B comprises backscattering in wire B only,

$$G_b^B\equiv\hat{A}_-[G_{\mathrm{wire}B}-G_{0-}]\ . \tag{34}$$

Now it is possible, in principle, to write down a series of all backscattering cycles in both wires. This procedure is straightforward but lacks elegance. Therefore we present immediately the desired expressions and justify them *a posteriori* in a rather heuristic way. We have

$$\tilde{f}^{AB}=\frac{f^-+f^-G_b^B\tilde{f}^{BB}}{1-f^+G_b^A} \tag{35}$$

and

$$\tilde{f}^{AA}=\frac{f^++f^-G_b^B\tilde{f}^{BA}}{1-f^+G_b^A}\ . \tag{36}$$

The corresponding scattering amplitudes $\tilde{f}^{BA}$ and $\tilde{f}^{BB}$ can be constructed by a simple change of the superscripts A and B. Each one of the expressions (35), (36) contains two constituents with different physical meaning. The first term comprises backscattering paths in wire A only and *excludes* any path into wire B, whereas the second one describes additional contributions from backscattering processes in wire B *after a first transmission* through the orifice. The higher-order transmissions via the hole are condensed in the renormalized scattering amplitudes of the second terms in Eqs. (35) and (36). We note that the symmetry relation $\tilde{f}^{AB}=\tilde{f}^{BA}$ holds.

Now we are going to consider the transmissivities T along wire A, and T_{AB} from wire A to B. Since the derivation of Eqs. (31) and (32) in the preceding section was based only on the transmission matrix t_{nm} within the wire they are applicable in the present case if the quantities belonging to the outer 2D space are replaced by those of the second wire. So the modified formulas read as

$$\begin{aligned}T_{AA}&=N-|\tilde{f}^{AA}|^2(\hat{A}_+\mathrm{Im}G_{\mathrm{wire}\,A})^2\\&\quad-2|\tilde{f}^{AB}|^2\hat{A}_-\mathrm{Im}G_{\mathrm{wire}B}\hat{A}_+\mathrm{Im}G_{\mathrm{wire}\ A}\end{aligned} \tag{37}$$

and

$$T_{AB}=2|\tilde{f}^{AB}|^2\hat{A}_+\mathrm{Im}G_{\mathrm{wire}\ A}\hat{A}_-\mathrm{Im}G_{\mathrm{wire}\ B}\ . \tag{38}$$

The corresponding quantities T_{BA} and T_{BB} are obtained again by a simple change of the indices A and B in (37) and (38). As we should expect from general symmetry relations,[3] $T_{AB}=T_{BA}$ holds exactly.

V. DISCUSSION AND NUMERICAL RESULTS

Now we will investigate how the various transmittivities found in Secs. III and IV depend on energy. For this purpose, we analyze the renormalized scattering amplitudes which enter all formulas.

We start at $T_{\rm wire}$ and $T_{\rm out}$ from Eqs. (31) and (32) for a single and possibly leaky wire. The typical denominator of $\tilde{f}^+$ and $\tilde{f}^-$, see Eq. (27),

$$D(k^2)=\mathrm{Re}\left[\frac{1}{f^+}-G_b\right] + i(\hat{A}_+\mathrm{Im}G_{\rm wire}+|f^-/f^+|^2\hat{A}_-\mathrm{Im}G_{0-})\ , \qquad (39)$$

is a quantity that shows a pronounced energy dependence around mode thresholds.[6–8]

Far enough from mode thresholds we have $\mathrm{Re}D(k^2)\approx\mathrm{Re}1/f^+$, cf. Refs. 7 and 8, and $\mathrm{Im}D(k^2)\sim 1$ [see the remarks after Eqs. (12) and (29)]. This means $\tilde{f}^+\approx f^+, \tilde{f}^-\approx f^-$, and thus

$$\begin{aligned} T_{\rm wire} &\approx N-|f^+|^2(\hat{A}_+\mathrm{Im}G_{\rm wire})^2 \\ &\quad -2|f^-|^2\hat{A}_+\mathrm{Im}G_{\rm wire}\hat{A}_-\mathrm{Im}G_{0-} \\ &\approx N \end{aligned} \qquad (40)$$

and

$$T_{\rm out}\approx 2|f^-|^2\hat{A}_+\mathrm{Im}G_{\rm wire}\hat{A}_-\mathrm{Im}G_{0-}\ll 1\ . \qquad (41)$$

This situation corresponds to the smooth parts of the curves in Fig. 2 which are given as illustration.

However, if the energy approaches the Nth mode threshold from below, the Nth term in the sum of $\mathrm{Re}\hat{A}_+G_{\rm wire}$ that enters $\mathrm{Re}G_b$, see Eq. (22), diverges as k_N^{-1} and outweighs all other terms such that

$$\mathrm{Re}G_b\approx\frac{N^2\kappa^2}{Lk^2k_N}\gg 1\ . \qquad (42)$$

If the perturbation is a convex bump or an orifice, i.e., $\mathrm{Re}1/f^+>0$, the divergence of $\mathrm{Re}G_b$ leads to $\mathrm{Re}D(k^2)=0$ at an energy $k^2_{\rm QBS}$ which is separated from the Nth threshold by

$$\begin{aligned} \Delta\equiv\kappa^2N^2-k^2_{\rm QBS} &\approx\left[\frac{N^2\kappa^2|f^+|}{Lk^2}\right]^2 \\ &\sim\kappa^2\left[\frac{a}{L}\right]^4\ , \end{aligned} \qquad (43)$$

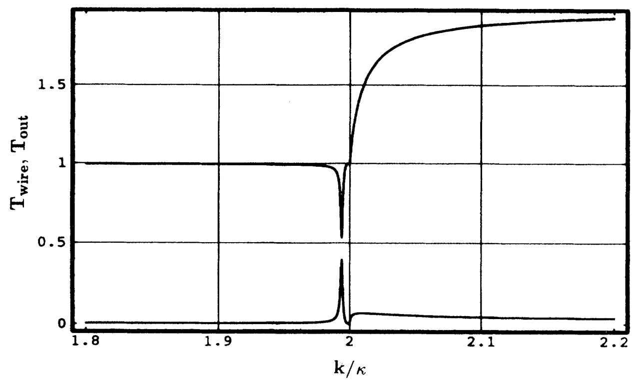

FIG. 2. The transmissivities $T_{\rm wire}$ (upper curve) and $T_{\rm out}$ (lower curve) vs k/κ around the second mode threshold. The orifice parameters are $a/L=0.1$ and $|f^-/f^+|^2=0.5$. The sharp resonances below each threshold are clear to see.

where in the second line the estimation of $|f^+|$ from Sec. II has been used. Additionally, we assume $N\sim 1$, i.e., not too many propagating modes. Such a resonance in $\tilde{f}^+$ and $\tilde{f}^-$ is called the quasibound state and has been discussed extensively for isolated scatterers.[6,8,33] It results in a peak of $|\tilde{f}^+|^2$ and $|\tilde{f}^-|^2$ with a height

$$\begin{aligned} |\tilde{f}^+_{\rm QBS}|^2 &= \frac{1}{(\hat{A}_+\mathrm{Im}G_{\rm wire}+|f^-/f^+|^2\hat{A}_-\mathrm{Im}G_{0-})^2}\ , \\ |\tilde{f}^-_{\rm QBS}|^2 &= \frac{|f^-/f^+|^2}{(\hat{A}_+\mathrm{Im}G_{\rm wire}+|f^-/f^+|^2\hat{A}_-\mathrm{Im}G_{0-})^2}\ , \end{aligned} \qquad (44)$$

and a width Γ of

$$\Gamma\equiv\left[\frac{\mathrm{Im}\dfrac{1}{f^+}}{\dfrac{d}{d(k^2)}\mathrm{Re}\dfrac{1}{\tilde{f}^+}}\right]_{k_{\rm QBS}}\sim\kappa^2\left[\frac{a}{L}\right]^6\ll\Delta\ . \qquad (45)$$

Γ can be interpreted as decay width of the quasibound state.[6,8,33] Now we can insert $|\tilde{f}^-_{\rm QBS}|^2, |\tilde{f}^+_{\rm QBS}|^2$ into Eqs. (31) and (32) and get the transmissivities at the QBS resonance:

$$T_{\rm wire}=N-\frac{(\hat{A}_+\mathrm{Im}G_{\rm wire})^2+2|f^-/f^+|^2\hat{A}_+\mathrm{Im}G_{\rm wire}\hat{A}_-\mathrm{Im}G_{0-}}{(\hat{A}_+\mathrm{Im}G_{\rm wire}+|f^-/f^+|^2\hat{A}_-\mathrm{Im}G_{0-})^2} \qquad (46)$$

and

$$T_{\rm out}=2\frac{|f^-/f^+|^2\hat{A}\,\mathrm{Im}G_{0-}\,\hat{A}\,\mathrm{Im}G_{\rm wire}}{(\hat{A}\,\mathrm{Im}G_{\rm wire}+|f^-/f^+|^2\hat{A}\,\mathrm{Im}G_{0-})^2}\ . \qquad (47)$$

For a closed bump, i.e., $f^-=0$, we get $T_{AA}\to N-1$, in analogy to isolated scatterers.[7,11] For a short orifice, i.e., $|f^-/f^+|^2\sim 1$, $T_{\rm out}$ is in the order of unity and thus the flux out of the wire represents an experimentally measurable quantity. Also these resonances are clear to see in Fig. 2.

On the contrary, for a long narrow opening, transmission out of the wire is exponentially small at QBS resonances inside the wire, while $T_{\rm wire}$ shows a dip down to $N-1$. Due to the smallness of the leakage flux, this case thus seems to be uninteresting from an experimental point of view and is therefore excluded furthermore from our considerations. However, it is surprising to find that even such a weak link to the outer space can influence the transport inside the wire considerably.

It is well known from isolated short-ranged scatterers[7,8,11] that the transmissivity along the wire shows downward dips, the depth of which does not depend on the strength of the scatterers. Here, we have shown this fact to be true also for closed surface scatterers. For orifices, the dip depth of $T_{\rm wire}$ as well as the peak height are ruled merely by the ratio $|f^-/f^+|^2$. The plots merely become sharper but reach the same height for smaller but geometrically similar orifices.

If the bump is concave, $\mathrm{Re}1/f^+<0$, no QBS is possible. Having in mind the work on isolated scatterers in a quantum wire, we point out the striking analogy between surface perturbations and volume scatterers: Orifices and convex bumps correspond to attracting impurities while concave bumps are comparable to repulsive scatterers.

Further, approaching a mode threshold *from below* leads to further divergence of $\mathrm{Re}D(k^2)$, see (42). Consequently, $\tilde f^+$, $\tilde f^-$ finally vanish and the transport along the wire becomes ballistic while the transmission through the small hole is inhibited.

If the energy approaches the Nth threshold *from above*, the quasi-one-dimensional LDOS belonging to this mode diverges, and so does $\hat A_+\mathrm{Im}G_{\rm wire}$. Thus, the renormalized scattering amplitudes become zero again. This yields $T_{\rm out}\to 0$. On the other hand, however, one could naively expect $T_{\rm wire}=N+1$ but the huge LDOS renders the wire extremely sensitive to any perturbation and just compensates the vanishing scattering amplitude. This results in $T_{\rm wire}\to N$. (A similar discussion for isolated scatterers can be found in Ref. 7.)

Finally we investigate a double-wire system by evaluating Eqs. (37) and (38). In general, these expressions are quite difficult to handle because they contain renormalized scattering amplitudes which are mutually coupled by Eqs. (36) and (35). However, we can simplify them if the mode thresholds of both wires are sufficiently separated from each other. In other words, this means that, if any, only the divergent backscattering amplitude or LDOS, respectively, of one wire must be taken into account whereas the other one can be neglected. Two thresholds n_A and n_B can be regarded as well separated in the above sense if

$$|\kappa^2_{\mathrm{wire}\,A}n_A^2-\kappa^2_{\mathrm{wire}B}m_B^2|\gg\Delta \tag{48}$$

because the typical denominator $D(k^2)$ departs remarkably from its normal value $\mathrm{Re}1/f^+$ only in an energy range of the order Δ around a mode threshold.[7] In the following, we will assume condition (48) to be valid. Our considerations of a wire couple are illustrated by Fig. 3.

If there is an enhanced backscattering in neither wire A nor wire B, all renormalized scattering amplitudes are approximately equal to their vacuum quantities, as discussed for the single wire case. Hence,

$$T_{AA}\approx N-|f^+|^2(\hat A_+\mathrm{Im}G_{\mathrm{wire}\;A})^2 -2|f^-|^2\hat A_+\mathrm{Im}G_{\mathrm{wire}\;A}\hat A_-\mathrm{Im}G_{\mathrm{wire}\;B}\approx N \tag{49}$$

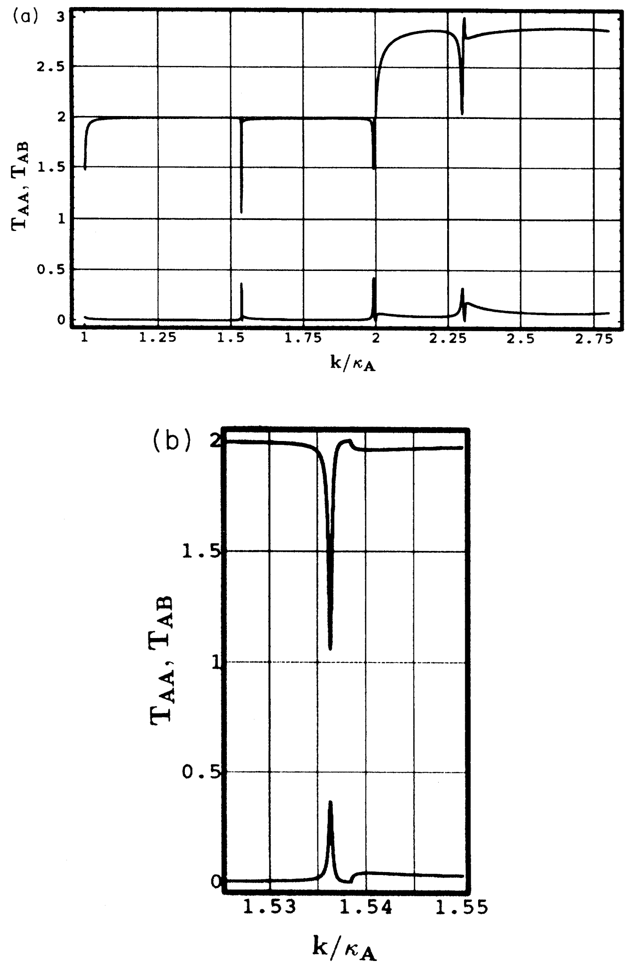

FIG. 3. The transmissivities T_{AA} (upper curve, shifted by unity) and T_{AB} (lower curve) vs k/κ_A for a coupled-wire system with the parameters $L_B/L_A=1.3$, $a/L_A=0.1$ and $|f^-/f^+|^2=0.8$. (a) Overall plot between the first and third threshold of wire A. The sharp dips of T and the corresponding peaks of T_{AB} are caused by quasibound states in either of the wires. (b) Detailed plot of the region around the second threshold of wire B. The QBS-caused dip in T_{AA} below the threshold is followed by the transparency peak on the threshold, as discussed after Eq. (54).

and

$$T_{AB}\approx 2|f^-|^2\hat A_+\mathrm{Im}G_{\mathrm{wire}\;A}\hat A_-\mathrm{Im}G_{\mathrm{wire}\;B}\ll 1\;, \tag{50}$$

cf. Eqs. (40) and (41).

However, if in one of both wires a QBS resonance is present, i.e., either $\mathrm{Re}(1/f^+-G_b^A)=0$ or $\mathrm{Re}(1/f^+-G_b^B)=0$ holds, a lengthy but principally simple analysis of $\tilde f^{AA}$ and $\tilde f^{AB}$ gives

$$T_{AA}=N-\frac{(\hat A_+\mathrm{Im}G_{\mathrm{wire}\;A})^2+2|f^-/f^+|^2\hat A_+\mathrm{Im}G_{\mathrm{wire}\;A}\hat A_-\mathrm{Im}G_{\mathrm{wire}\;B}}{(\hat A_+\mathrm{Im}G_{\mathrm{wire}\;A}+|f^-/f^+|^2\hat A_-\mathrm{Im}G_{\mathrm{wire}\;B})^2} \tag{51}$$

and

$$T_{AB}=2\frac{|f^-/f^+|^2\tilde{A}_-\mathrm{Im}G_{\mathrm{wire}\ B}\hat{A}_+\mathrm{Im}G_{\mathrm{wire}\ A}}{(\tilde{A}_+\mathrm{Im}G_{\mathrm{wire}\ A}+|f^-/f^+|^2\hat{A}_-\mathrm{Im}G_{\mathrm{wire}\ B})^2}\ . \tag{52}$$

Note that it plays no role at all when backscattering of both wires leads to a quasibound state. It is the bare existence of a QBS that gives rise to this enhanced coupling. Note these resonances in Fig. 3.

Further approaching a mode threshold of wire A from below leads to transparency of wire A again and inhibits the coupling between the wires. In full analogy to the single leaky wire, approaching a mode threshold of A from above inhibits the transmission through the orifice, while the transmissivity along this wire is decreased from its ballistic value by unity due to the diverging LDOS of wire A.

On the other hand, if the energy equals a mode threshold of wire B, an analysis of $\tilde{f}^{AA}$ and $\tilde{f}^{AB}$ for the special case $G_b^B\to\infty$ gives

$$\tilde{f}^{AB}\to 0,\quad \tilde{f}^{AA}\to f^+(1-(f^-/f^+)^2)\ , \tag{53}$$

and thus

$$T_{AB}\to 0, \tag{54}$$

$$T\to N-(\hat{A}_+\mathrm{Im}G_{\mathrm{wire}\ A})^2|f^+|^2|1-(f^-/f^+)^2|^2\ .$$

It is interesting to find here that for short orifices, i.e., $(f^-/f^+)^2\sim 1$, wire A becomes nearly ballistic. We interpret this by the fact that backscattering paths into B return to A without real phase shift because the wave fits exactly into B. Thus, it is indistinguishable for wire A whether B is present or not. Such a peak is found twice in Fig. 3(a). Since the one at the second threshold of wire B is very sharp, a zoom plot is given in Fig. 3(b).

On the contrary, if the coupler is very long, both wires can be regarded as independent ones. The resonance of B does not affect wire A.

VI. CONCLUSIONS

In this paper, we have studied the influence of a short-ranged boundary irregularity in a quantum wire on transport. We considered closed bumps and openings as well.

One of the tools we have used is the optical theorem. Its usefulness in the description of scattering problems, especially in the simplification of various expressions for transport quantities, has been shown in previous papers. Here, we have derived it for surface scatterers.

The transport behavior inside a wire in the presence of a convex boundary perturbation which couples the wire to free space very weakly or is even closed was shown to be qualitatively the same as for isolated scatterers in the wire.[7,8,11] Quasibound states lead to sharp dips in the transmissivity along the wire.

The transmissivity out of the wire for long narrow openings exhibits narrow but exponentially small peaks at QBS energies below a mode threshold of the wire. The investigation of such long narrow couplers that could serve as a model for a weakly coupling probe shows that at singular energies the bare presence of a surface perturbation strongly affects the transport inside the wire without respect to the strength of coupling.

In the opposite case of short couplers, the transmissivity from inside to outside the wire shows narrow peaks in the order of unity, whereas the transmissivity along the wire is decreased to a value between $N-1$ and N. They should be measurable in an appropriate experimental setup.

If two wires are coupled with each other, then the interplay of backscattering in both wires gives rise to very complex expressions for the renormalized scattering amplitudes. We have shown that it is possible to decompose those complicated formulas for the case that both wires have different widths such that resonances in both wires do not overlap. Using these simplifications, we have considered off-resonant and resonant coupling between both wave guides. Resonant coupling occurs when a QBS in one or both wires is present and results in narrow transmissivity peaks that are on the order of unity if the connection is of the short type. This effect should be detectable in experiments, too. It is similar to interference effects proposed recently by Price[28] and Porod, Shoa, and Craig[29] for a resonator attached to a wire. We believe our method to be appropriate for a detailed investigation of the phenomena discussed there.

It is worthwhile to remark that the peak heights of the coupling transmissivities depend only on the ratio of the scattering amplitudes of the opening, $|f^-/f^+|^2$. Merely the energetic position and the width of the QBS resonances depend strongly on the single quantity f^+.

In conclusion, we find the language of multiple scattering and renormalized scattering amplitudes to be well suited to problems like this. Starting from LDOS and scattering amplitudes, it was possible to analyze the present transport problem in an analytical way. The method presented here for two dimensions can be applied also in three-dimensional structures because the multiple-scattering approach with its, in principle, simple concept is not restricted to a special dimensionality.

We also hope that this paper will stimulate some further experiments.

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[1] B. J. van Wees, H. van Houten, C. W. J. Beenakker, J. G. Williams, L. P. Kouwenhowen, D. van der Marel, and C. T. Foxon, Phys. Rev. Lett. **60**, 848 (1988).

[2] D. A. Wharam, T. J. Thornton, R. Newbury, M. Pepper, H. Ritchie, and G. A. C. Jones, J. Phys. C **21**, L209 (1988).

[3] M. Büttiker, *Semiconductors and Semimetals* (Academic, New York, 1992), Vol. 35, Chap. 4.

[4] M. Büttiker, IBM J. Res. Dev. **32**, 317 (1988).

[5]E. Tekman and S. Ciraci, Phys. Rev. B **43**, 7145 (1991).
[6]Y. B. Levinson, M. I. Lubin, and E. V. Sukhorukov, Phys. Rev. B **45**, 11 936 (1992).
[7]Ch. Kunze and R. Lenk, Solid State Commun. **84** 457 (1992).
[8]M. I. Levinson, Y. B. Lubin, E. V. Sukhorukov, and Ch. Kunze (unpublished).
[9]Ch. Kunze, Proceedings of the 7th International Conference of Physics Students (International Association of Physics Students, Lisbon, 1992).
[10]Ph. F. Bagwell, Phys. Rev. B **41**, 10 354 (1990).
[11]C. S. Chu and R. S. Sorbello, Phys. Rev. B **40**, 5941 (1989).
[12]A. Kumar and Ph. F. Bagwell, Phys. Rev. B **43**, 9012 (1991).
[13]A. Kumar and Ph. F. Bagwell, Phys. Rev. B **44**, 1747 (1991).
[14]R. Lenk, Phys. Status Solidi B **161**, 797 (1990).
[15]R. Lenk, Phys. Status. Solidi B **162**, 227 (1990).
[16]J. Faist, P. Guèret, and H. Rothuizen, Phys. Rev. B **42**, 3217 (1990).
[17]J. Faist, P. Guèret, and H. Rothuizen, Superlatt. Microstruct. **7**, 349 (1990).
[18]G. Timp, R. E. Behringer, and J. E. Cunningham, Phys. Rev. B **42**, 9261 (1990).
[19]Y. B. Levinson and E. V. Sukhorukov, Phys. Lett. A **149**, 167 (1991).
[20]A. Matulis and K. Patieunas, J. Phys. Condens. Matter **3**, 5543 (1991).
[21]T. Ando and H. Tamura, Phys. Rev. B **46**, 2332 (1992).
[22]N. M. Makarov and I. V. Jurkevitch, Zh. Eksp. Teor. Phys. **96**, 1106 (1989) [Sov. Phys. JETP **69**, 628 (1989)].
[23]J. Lekner, *Theory of Reflection* (Martinus Nijhoff, Dordrecht, 1987).
[24]F. G. Bass and I. M. Fuks, *Wave Scattering by Statistically Rough Surfaces* (Pergamon, Oxford, 1979).
[25]A. Sommerfeld, *Partial Differential Equations in Physics* (Academic, New York, 1949).
[26]Y. Takagaki and D. K. Ferry, Phys. Rev. B **45**, 12 152 (1992).
[27]C. C. Eugster and J. A. del Alamo, Phys. Rev. Lett. **67**, 3586 (1992).
[28]P. J. Price, IEEE Trans. Electron Devices **39**, 520 (1992).
[29]W. Porod, Zhi an Shoa, and S. Lent Craig, Appl. Phys. Lett. **61**, 1350 (1992).
[30]R. L. Schult, D. G. Ravenhall, and H. W. Wyld, Phys. Rev. B **39**, 5476 (1989).
[31]V. V. Paranjape, J. Phys. Condens. Matter **3**, 6715 (1991).
[32]Yu. B. Gaididei, L. I. Malysheva, and A. I. Onipko, Phys. Status Solidi B **172**, 667 (1992).
[33]Ch. Kunze, Y. B. Levinson, M. I. Lubin, and E. V. Sukhorukov, Pis'ma Zh. Eksp. Teor. Fiz. **56**, 56 (1992) [JETP Lett. **56**, 55 (1992)].
[34]Ch. Kunze (unpublished).
[35]P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (MacGraw-Hill, New York, 1953).
[36]L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Pergamon, Oxford, 1977).