Circular bends in electron waveguides

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We study the scattering properties of bends in two-dimensional electron waveguides. We focus on a circular bend model in which the shape of the bend is determined by the bending angle and the ratio between the internal radius and the width of the asymptotic perfect leads. Such a geometry is assumed to be delimited by hard-wall boundaries. The transmission probability between the various incoming and outgoing transverse modes is studied as a function of the electron energy and the bend geometry. The total transmission probability is practically unity except at energies very close to the mode propagation thresholds. The span of the energy intervals where reflection is finite increases with the bend internal curvature. A circular bend can be a powerful mode convertor, as revealed by the rich structure of the mode-resolved transmission probabilities, which are periodic or quasi-periodic functions of the bending angle and display decaying oscillations as a function of the radius. We also show that one or more bound states exist in a circular bend and calculate their binding energy for various bend geometries. A brief discussion of the analogy between electron and electromagnetic waveguides is provided.

Recent progress in nanostructure technology has made possible the fabrication of semiconductor structures whose size is smaller than the carrier elastic and inelastic mean free path.[1] In such a ballistic regime, the boundaries defining the geometry of the structure constitute the only source of scattering. If the wavelength of the Fermi electrons is comparable to the dimensions of the sample and in particular to the width of the leads, it is appropriate to view a quantum wire as an electron waveguide in which the quantization of the transverse motion plays an important role.[2,3] The prospect of building devices based on electron waveguide properties is opening an exciting area of research within the physics of semiconductor devices.[4,5] In this context, it is of interest to understand various aspects of electron transport in narrow wires. An understanding of the role of geometry in nanostructures will be of increasing importance as electron waveguide networks become a reality. This paper addresses the problem of the role played by bends in electron waveguides, which one expects to be ubiquitous in ultrasmall semiconductor structures. The study we present here complements previous work on scattering by boundaries in electron waveguides.[4-10] We study the hard-wall boundary geometry shown in the inset of Fig. 1, where two perfect leads aligned in different directions are connected smoothly by a central region delimited by concentric boundaries of constant curvature. While this model for the bend probably tends to underestimate the resistance to the current flow posed by real bends, it complements models of bends formed by abrupt corners which presumably overestimate such resistance. The circular bend model has the additional advantage of permitting a simple treatment of the bending angle and the radius of curvature as continuous variables.

Since the early work of Landauer,[11] it has been known that the contribution to the resistance by a given obstacle is closely related to its electron scattering properties. In recent years, this connection between the *I-V* response and the scattering amplitudes has been refined and generalized to more arbitrary mesoscopic structures.[12-15] It has been recognized that this relation between scattering and resistance is not necessarily unique and may depend on the experimental arrangement and the choice of voltage references. In the present work, we treat the bend as an effective impurity and focus on the scattering problem posed by the structure of Fig. 1. We do not enter here into the more general discussion on the relation between resistance and transmission probabilities.[12,15] For a given wire width W, the shape of the bend is determined by the internal radius ρ_0 and the bending angle θ. We want to calculate the transmission and reflection coefficients between various transverse modes (channels) as a function of the electron energy E and the geometrical variables θ and ρ_0/W. We employ here a wave-function matching method which is similar to that employed by Schult *et al.*[9] to study electron scattering at crossed wires. Recently, Frohne *et al.*[16] have developed a general matching method to study the scattering by boundaries in arbitrary geometries. In addition to the scattering calculation, we show that one or more bound states nucleate at a bend and calculate its binding energy for a number of cases.

It is appropriate to make some remarks here on the extent of the analogy between the thoroughly studied electromagnetic waveguides[17] and the relatively unexplored electron waveguides. We are interested in their similarity as problems in mathematical physics. The scattering by discontinuities depends quantitatively on the set of available transverse modes, since in general all of them become involved in the wave matching process. The presence of transverse-electric (TE) and transverse-magnetic (TM) modes in electromagnetic waveguides precludes a complete mathematical analogy between these and the relatively simpler electron waveguides. However, in a very flat rectangular electromagnetic waveguide (i.e., one for which $b \ll a$, where a and b are the dimensions of the rectangular cross section) the high cutoff frequency of the TM and TE_{mn} (with $n \neq 0$) modes leaves the TE_{m0} modes as the only active modes in the propagation and scattering processes.[17] The set of TE_{m0} modes in a waveguide with perfectly conducting walls is isomorphic to the set of transverse modes in a two-dimensional hard-wall electron waveguide (which in turn must also be viewed as a limiting case of a very flat three-dimensional waveguide in wich the electron motion in one direction is completely frozen). It can therefore be said that two-dimensional electron waveguides are mathematically equivalent to very flat rectangular electromagnetic waveguides. Such a limiting type of waveguide is, however, not particularly interesting from the engineering viewpoint and, to the best of our knowledge, it has not been studied in detail. There is of course a general qualitative similarity between electromagnetic waveguides and their new electron counterparts. In this sense, the novel field of nanostructures physics can benefit substantially from the already existing experience in waveguide design.[17]

We wish to solve the two-dimensional Schrödinger equation for an electron moving in a potential which is zero in regions I, II, and III of Fig. 1 (inset) and infinite elsewhere (motion in the third dimension is assumed to be

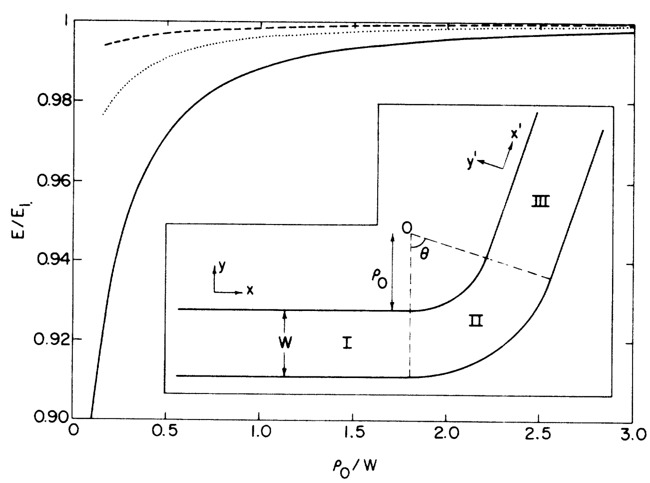

FIG. 1. The energy threshold for propagation within the bend in the fundamental mode (solid line) and the bound-state energies for bends of 90° (dashed) and 180° (dotted) are plotted as a function of the bend radius in reduced units. Inset: schematic picture of the circular bend model studied in this paper.

completely frozen). In the perfect leads I and III, the most general wave function for an electron with energy E is of the form

$$\psi_{\mathrm{I}}(\boldsymbol{\rho})=\sum_{n=1}^{\infty}\chi_n(y)(a_n e^{k_n x}+e_n e^{-k_n x}) , \tag{1a}$$

$$\psi_{\mathrm{III}}(\boldsymbol{\rho})=\sum_{n=1}^{\infty}\chi_n(y')(b_n e^{-k_n x'}+f_n e^{k_n x'}) , \tag{1b}$$

where $\chi_n(y)=(2/W)^{1/2}\sin(N\pi y/W)$ is the wave function for transverse motion in mode n and $k_n^2=(n\pi/W)^2-2ME/\hbar^2$. For evanescent modes ($k_n^2>0$), we set $k_n=|k_n|$, which requires $e_n=f_n=0$. For asymptotically propagating modes ($k_n^2<0$), we have $k_n=-i|k_n|$, so that e_n and f_n are the amplitudes of the incoming waves while a_n and b_n are those of the outgoing waves.

In region II, the Schrödinger equation can be separated when it is written in polar coordinates (see inset of Fig. 1): ρ is the distance to point 0 and ϕ is the angular coordinate whose origin lies at the I-II interface and which grows counterclockwise. For solutions of the type $\phi(\boldsymbol{\rho})=P(\rho)\Phi(\phi)$, the Schrödinger equation becomes

$$\frac{d^2\Phi(\phi)}{d\phi^2}=\nu^2\Phi(\phi) , \tag{2a}$$

$$\rho^2\frac{d^2P(\rho)}{d\rho^2}+\rho\frac{dP(\rho)}{d\rho}+\rho^2k^2P(\rho)=-\nu^2P(\rho) , \tag{2b}$$

where $k^2=2ME/\hbar^2$. Thus, the most general solution in region II has the form

$$\psi_{\mathrm{II}}(\boldsymbol{\rho})=\sum_{n=1}^{\infty}P_n(\rho)(c_n e^{\nu_n\phi}+d_n e^{-\nu_n\phi}) , \tag{3}$$

where $P_n(\rho)$ and ν_n are solutions of the eigenvalue equation (2b) *for a given energy E*, subject to the hard-wall boundary conditions $P_n(\rho_0)=P_n(\rho_0+W)=0$. These solutions define the possible modes of propagation within the bend. In analogy to the convention for perfect leads, the case $\nu_n=|\nu_n|$ corresponds to an evanescent mode, while $\nu_n=i|\nu_n|$ yields a propagating mode with angular momentum $\hbar|\nu_n|$.

The matching conditions are determined by the requirement of continuity of the wave function and its normal derivative at the interfaces I-II and II-III. If the infinite sums in (1) and (3) are truncated at N terms, the four continuity equations (two for each interface) become a set of $4N$ coupled homogeneous linear equations in the coefficients a_n, b_n, c_n, d_n, e_n, and f_n, after they are projected on the N transverse modes $\chi_n(y)$. Such a system of equations can be written in the form $M_{ij}u_j=v_i$, where u_i is a vector whose $4N$ components are the coefficients a_n, b_n, c_n, and d_n for the outgoing and internal bend waves [see Eqs. (1) and (3)]. The $4N$ component vector v_i contains the amplitudes e_n and f_n of the incoming waves (each coefficient appears twice). M_{ij} is a $4N\times4N$ matrix that contains the information on the matching conditions at the interfaces. For a bound state, all the modes are evanescent in the perfect leads, so that $e_n=f_n=0$. Thus, the energy of a bound state satisfies the equation

$\det M = 0$. For the calculation of the S matrix (formed by the transmission and reflection coefficients) one must invert the matrix M, since the equation $u = M^{-1}v$ yields the amplitudes of the outgoing waves in terms of those of the incoming waves (proper care has to be taken of the velocity of propagation in the different transverse modes).

It is interesting to note that the energy thresholds for propagation are lower in the bend than they are in the perfect leads. As an example, we show in Fig. 1 the energy threshold for propagation in the first angular mode, which is obtained by setting $\nu_1^2 = 0$. For large radius (flat limit) this threshold tends asymptotically to $E_1 = \hbar^2\pi^2/2MW^2$, which is the minimum energy for propagation in the fundamental mode along the perfect wires. A very similar curve is obtained for the thresholds of higher angular modes if these are referred to the corresponding straight wire values, $E_n = n^2E_1$. Therefore, one can view the bend as a resonator whose effective width is slightly larger than that of the waveguide in which it is introduced. The larger effective width accounts for the lower minimum energy for propagation. The effective length of the resonator is proportional to the bending angle. This resonator analogy permits a qualitative understanding of some properties of circular bends. A good example is the existence of a bound state, which one can expect to find at energies between the thresholds for propagation in the bend and in the perfect lead. In Fig. 1, the energy of the bound states at bends of angles 90° and 180° are plotted as a function of the internal radius (at artificially large angles, more than one bound state may develop). It is clear that the binding energy $E_1 - E_{BS}$, decreases with increasing radius and with decreasing angle. This is consistent with what will be seen for the electron transmission: the effective scattering strength of a circular bend tends to decrease for large radius and small angle. These states are more weakly bound than the bound state at an L-shaped bend with sharp right angle corners. In that case $E_{BS} = 0.92E_1$,[9] to be compared with, e.g., $E_{BS} = 0.97E_1$ for $\rho_0 = 0.15W$ and $\theta = 180°$. (We have not plotted the bound-state energies at smaller radii because in that regime our numerical algorithm becomes less reliable; however for $\rho_0 \to 0$ we can expect E_{BS} to tend to a finite value which should be somewhat higher than the corresponding level of an L-shaped bend).

In Fig. 2 we show several electron transmission probabilities as a function of the electron energy for bending angle $\theta = 90°$ and internal radii $\rho_0/W = 0.2$ and 0.5. T_{nm} is the probability that an incident electron in mode n is transmitted into mode m (note that, due to the symmetries of time reversal and reflection around the axis $\phi = \theta/2, T_{nm} = T_{mn}$). For the propagating modes considered, ($n = 1,2,3$) the total transmission $T_n = \sum_m T_{nm}$ is practically unity at all energies except very close to the thresholds E_n. The conclusion is that these ideal circular bends introduce almost no additional resistance to the current flow except in those cases where energy happens to lie very close to one of the mode thresholds.

The transmission probabilities $T_{nm}(E)$ undergo very rapid variations just below the threshold energies E_n. This is a signature of the presence of resonances, whose nature is similar to that of the bound state below E_1 mentioned above.[7,9] They can be viewed as quasibound states of the subband whose threshold lies just above them. The finite width of these resonances comes from their coupling to the continuum of states in lower subbands. The effect of resonances on the transport properties of crossed narrow conductors has been recently studied by Kirczenow[7] in connection with the quenching of the quantum Hall effect. In the case of circular bends, we have found that, for the ratio $\rho_0/W = 0.2$ [Fig. 2(a)], there is a resonance of width ≈ 0.001 and binding energy ≈ 0.006 (in units of E_1) below the threshold for $n = 3$. Not shown in Fig. 2(a), T_{11} presents a dip of width $\approx 0.005E_1$ at a similar distance below E_2 in which the transmission goes all the way to zero. Due to the exceedingly small scale of energies, we do not expect these resonances to be of experimental relevance in most practical cases.

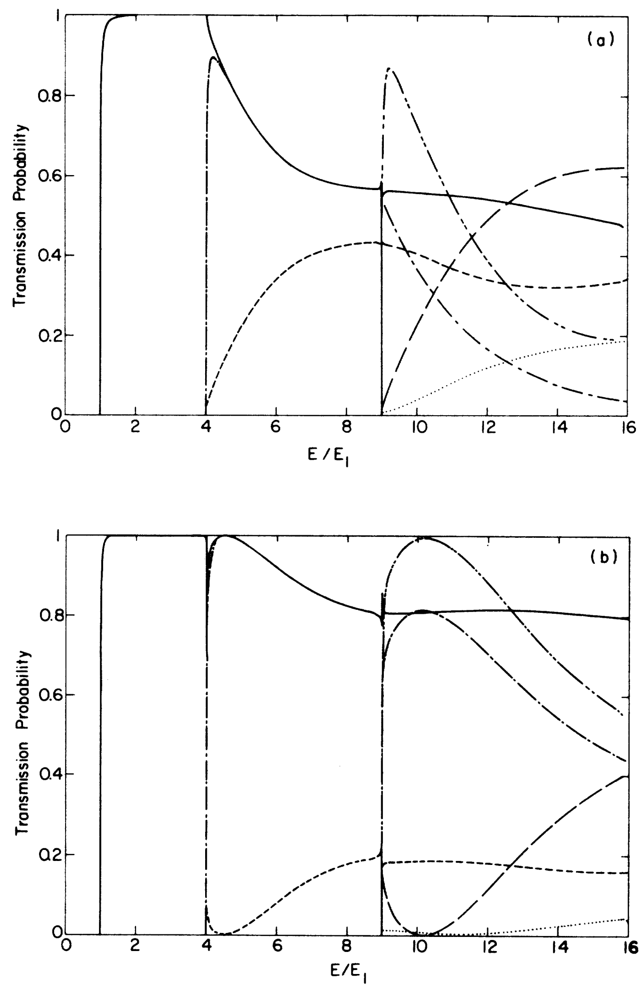

FIG. 2. Transmission probabilities T_{nm} between transverse modes n and m plotted as a function of energy for a bend of 90° and internal radius (a) $\rho_0 = 0.2W$ and (b) $0.5W$: T_{11} (solid), T_{12} (short dashed), T_{13} (dotted), T_{22} (dot-dashed), T_{23} (long-dashed), and T_{33} (double chain dotted). Note that $T_{nm} = T_{mn}$.

Although there is total transmission in the vast majority of situations, Fig. 2 shows that there is a rich structure in the conversion of modes. The probability that the electron changes mode increases with energy in most of the cases considered, while the probability $T_{nn}(E)$ of remaining in the same modes decreases after a rapid increase just above E_n. For a given energy the probability of mode conversion is quite sensitive to the shape of the bend. This can be appreciated in Fig. 3, where T_{11} and T_{12} are plotted as a function of ρ_0/W for several energies. T_{12} tends to decrease for large radii in a nonmonotonous manner. The length scale of the decaying oscillations increases with energy and (not shown here) decreases with the bending angle. After some careful considerations, this behavior can be understood in terms of the resonator analogy. The lack of interference between propagating modes gives rise to a poor structure of $T_{11}(\rho_0)$ for $E/E_1=1.05$. The sharp rise of $T_{11}=T_1$ at low ρ_0 is still more pronounced at higher energies within the single channel regime. Both the results on binding energies (Fig. 1) and the results on transmission probabilities reveal a decrease of the bend effective scattering strength at large radii. This trend can be understood in two complementary ways. As the bend radius increases, the structure of longitudinal and transverse modes becomes very close to that of the modes in the perfect wire. Therefore, at the perfect wire-bend interface, a given straight wire transverse mode is mostly converted into its closely resembling bend counterpart. On the other hand, one can also note that at large radii the electron wave adapts adiabatically to changes in the geometry that vary slowly in the wavelength scale and thus the reflection and mode conversion probabilities decrease. The importance of the concept adiabatic propagation in electron waveguides has been recognized in recent studies on the quenching of the low-field Hall resistance in quasi-one-dimensional ballistic microstructures.[8]

The interference patterns can best be observed in Fig. 4, where the transmission probabilities are plotted as a function of the bending angle θ for $\rho_0/W=0.2$ and

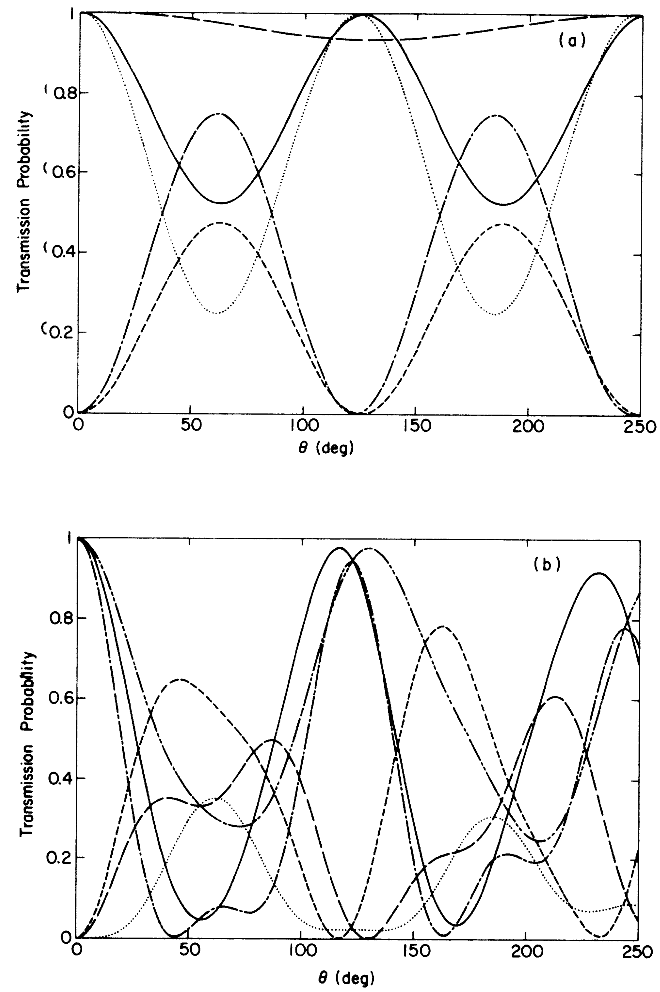

FIG. 4. Transmission probabilities as a function of the bending angle for a bend of radius $\rho_0=0.2W$. (a) For $E/E_1=5.5$ and 7.5, same convention as in Fig. 3. Here the long-dashed line stands for $E/E_1=1.1$. (b) For $E/E_1=12$, same convention as in Fig. 2.

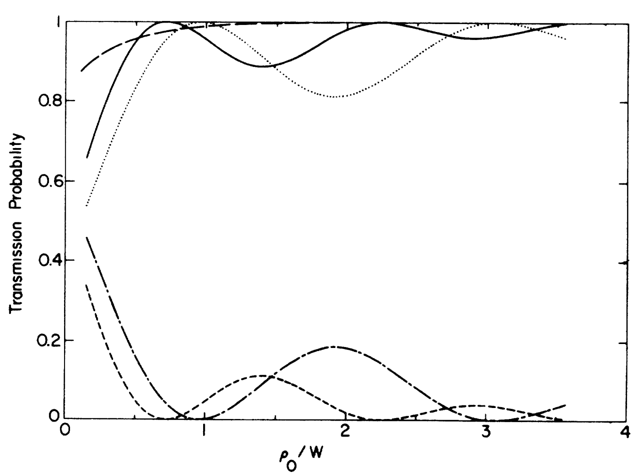

FIG. 3. Transmission probability T_{11} plotted as a function of the internal radius for $\theta=90°$ and $E/E_1=1.05$ (long dashed), 5.5 (solid), and 7.5 (dotted). T_{12} is shown for $E/E_1=5.5$ (short dashed) and 7.5 (dashed dotted).

$E/E_1=1.1$, 5.5, 7.5, and 12 (of course the range $\theta>180°$ lacks physical relevance but we included it for greater clarity). When more than one mode is available for propagation within the bend, the mode conversion is mainly determined by the interference between those propagating modes. This yields an oscillatory pattern in $T_{nm}(\theta)$ for $E/E_1=5.5$ and 7.5. The fact that the period increases with energy can be understood by noting that it is the difference between angular momenta that determines the interference and that this difference tends to decrease with increasing energy. To make this plausible it is illustrative to consider the flat limit ($\rho_0/W\to\infty$), where $\nu_n(E)=\pi(\rho_0/W)(E/E_1-n^2)^{1/2}$ and $(\nu_{n+1}-\nu_n)\propto E^{-1/2}$ for $E\gg n^2E_1$. For $E/E_1=1.1$, $T_{11}(\theta)$ has a period of about 250°. Unlike the single and double channel cases the presence of three propagating modes at $E=12E_1$ gives rise to a more complex quasiperiodic structure in $T_{nm}(\theta)$.

In conclusion, we have studied the scattering properties of a circular bend in an electron waveguide as a function of the electron energy and the geometry of the bend. We have found that the total transmission (summed over outgoing transverse modes) is practically unity almost everywhere in parameter space except at energies very close to the thresholds. The span of these energy regions with finite reflection increases with the internal curvature of the bend. In contrast with these results for the total transmission probability, we find that, for energies above the single channel regime, the mode resolved transmission probabilities T_{nm} present a strong dependence on E, θ, and ρ_0/W. The probability for mode conversion displays periodic or quasiperiodic oscillation as a function of the bending angle, and present strong oscillations as a function of the internal radius whose amplitude vanish at large radii. We have found that one or more bound states nucleate at a circular bend. Their binding energy is generally small except at strongly curved bends, in consistency with the effective scattering strength that is inferred from the results for mode-averaged transmission probabilities.

Note added in proof. We have recently learned that a similar study based on a different method but leading to the same main conclusions has been independently performed by Lent.[18]

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