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Quantum point contacts with smooth geometries: Exact versus approximate results

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Transport through quantum point contacts (QPC's) with various geometries close to those used experimentally is studied in the ballistic regime. We neglect impurity and temperature effects in an effort to understand the detailed status, as a function of geometry, of various popular approximations in this field, namely, the local adiabatic, the global adiabatic, and the diagonal approximation. By appeal to a combination of two well-known procedures, we are in a position to study, by exact numerical solution, continuous but rapidly varying geometries of QPC's. Our calculations show that the diagonal approximation is unreliable (as found previously by Castaño and Kirczenow). The local adiabatic approximation (Glazman *et al.*) can serve as a rough estimate, but significantly underestimates the sharpness of conductance steps. The global adiabatic approximation is remarkably successful, in spite of strong mode mixing. However, this approximation can also significantly underestimate the degree of conductance quantization. The physical reason for this is given. Resonance effects in continuous QPC's are found that confirm our physical interpretation.

I. INTRODUCTION

In 1988 two independent experimental groups[1,2] made the remarkable discovery that the conductance through a narrow constriction in a two-dimensional electron gas (2DEG) is quantized. The essential mechanism basic to this fact was immediately recognized: Transverse quantization allows propagation of a discrete set of modes through a "quantum point contact" (QPC) and, as follows from the Landauer-Büttiker formalism,[3] each such (spin degenerate) "channel" contributes $2e^2/h$ to the conductance. A more detailed understanding of the phenomenon,[4] including the shape of the conductance steps, involves the precise geometry of the QPC and, in addition, the influence of disorder and of temperature. In this paper we shall limit ourselves to some remarks in the final section on disorder and temperature effects, and concentrate on exact and approximate descriptions of transport through QPC's with various geometries. Many-body effects are neglected throughout.

The literature on this subject is quite extensive. It would be an exaggeration to call the problem a controversial one. Nevertheless, different viewpoints with somewhat conflicting conclusions do exist, and we hope to contribute to the clarification of some fundamental issues in this context by presenting a detailed comparison between several popular approximations and "exact" numerical results on the conductance of QPC's. For example, we demonstrate that exact calculations, when they differ, give better conductance quantization than the approximations used and, furthermore, we pinpoint the physical mechanism responsible for this effect.

The comparison has been made possible by the introduction of a combination of two standard numerical schemes in this field. On the one hand, the recursive Green function technique[5] applied to tight binding models has the important virtue of numerical stability, in addition to being quite flexible. Its weakness in this context is associated with the fact that the geometry must be discretized. This makes it difficult to model smoothly varying QPC's, since the transverse number of sites, N, associated with the widest part of the geometry determines the dimension of the matrices ($N \times N$) to be inverted. With a large number of inversions necessary one is, in practice, limited to $N \lesssim 100$. Alternatively, one can choose to work with exactly determined (local) transverse energy eigenstates. This reduces the problem to M coupled equations, with M typically of the order of 10. In this approach smoothness is no problem (on the contrary) and the dimension of the function space required for a realistic discussion is easily managed. However, the standard method for solving such coupled equations (after discretization of the longitudinal direction) is the transfer matrix method, or refinements thereof. These methods have numerical stability problems sufficiently serious to make a detailed discussion of a range of QPC's difficult. Our novel combination takes advantage of the strengths of both methods, while avoiding their weaknesses: We use the transverse energy modes as a basis, and can thereby handle smoothly varying geometries by a function space of reasonable dimensionality. On the other hand, we use the recursive Green function technique in the (discretized) longitudinal direction to determine the scattering matrix. Some further details of the method are given in the Appendix. The discussion of the QPC's in the sections below demonstrates the usefulness of our numerical scheme.

The paper is organized as follows. In Sec. II we recall what we shall denote the *local* adiabatic approximation, introduced by Glazman *et al.*,[6] and present the set of coupled equations on which two further approximations, which we shall refer to as the *global* adiabatic and the *di-*

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agonal one can be defined. This set of coupled equations also forms the basis on which our exact numerical work is done. In Sec. III an initial comparison is made between the three approximations and the exact results for the conductance of two typical QPC's. We then suggest a qualitative picture which explains these and subsequent results. Next, numerical results are presented for the conductance of a QPC with a shape very siniilar to that used by van Wees *et al.*[1] We also briefly discuss geometry induced resonances. Concluding remarks constitute Sec. IV.

II. BASICS

The two-point conductance through a QPC is given by the linear Landauer-Büttiker formula[3,5]

$$G = \frac{2e^2}{h} \sum_{\alpha,\beta} |t_{\alpha\beta}|^2 = \frac{2e^2}{h} \mathrm{Tr}\, tt^\dagger, \tag{1}$$

where $t_{\alpha\beta}$ is the transmission amplitude from incoming mode β to transmitted mode α, and spin degeneracy has been assumed. This formula gives, in principle, the conductance of a QPC connecting two infinite reservoirs. In our calculations we shall take the modes as those propagating in the leads. One could worry about the validity of the linear expression (1) in this context, with reference to the extended discussion on nonlinear versus linear formulas for the conductance, connected with probes in the leads versus in (infinitely) wide reservoirs.[4,7] We have checked that the leads used in our calculations are sufficiently wide that they can be considered as reservoirs, i.e., further widening of the leads has a negligible influence on the results. In other words, we can interpret our results, based on (1), for QPC's with leads of moderate width, as applying to the corresponding QPC's between infinite reservoirs.

The *local* adiabatic approximation was introduced by Glazman *et al.*[6] These authors consider only what happens in the narrowest part of the constriction, and assume that the influence of the widening areas is negligible as far as the conductance is concerned. As a result, the transmission probability only depends on the curvature R of the constriction at minimum width, and the minimum width W_0 itself. The resulting conductance can be written as

$$G = \frac{2e^2}{h} \sum_{\alpha} \frac{1}{1+\exp(-z_\alpha \kappa)}\ , \tag{2}$$

where $z_\alpha = (k_F W_0/\pi) - \alpha$ and $\kappa = \pi^2\sqrt{2R/W_0}$ with κ assumed larger than unity. Here α is the integer quantum number of the transverse mode, $k_F = \sqrt{2m^* E}/\hbar$ is the Fermi wave number, m^* the effective mass, and E the energy. An important advantage of this approximation is that it provides an analytic expression for the conductance as a function of energy. However, as we shall see, for geometries with rapid variations, like the QPC's typically used in experiments, the local adiabatic approximation compares rather unfavorably with exact calculations and has, at best, semiquantitative significance.

A *global* treatment of the transport problem starts from an expansion of the complete wave function in terms of local transverse energy eigenfunctions, $\Psi(x,y) = \sum_\alpha \chi_\alpha(x)\phi_\alpha(y;x)$, where we have chosen y as the transverse and x as the longitudinal direction. Inserting this expansion of the wave function into the Schrödinger equation, one obtains the following coupled differential equations for the mode coefficients,[8–10] $\chi_\alpha(x)$:

$$\left[E - E_\alpha(x) + \frac{\hbar^2}{2m^*}\frac{d^2}{dx^2}\right]\chi_\alpha(x) = -\frac{\hbar^2}{2m^*}\sum_\beta \left[2A_{\alpha\beta}(x)\frac{d}{dx} + B_{\alpha\beta}(x)\right]\chi_\beta(x), \tag{3}$$

where $\phi_\alpha(y;x)$ satisfies the (local in x) transverse Schrödinger equation

$$\left[-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial y^2} + V(y;x)\right]\phi_\alpha(y;x) = E_\alpha(x)\phi_\alpha(y;x) \tag{4}$$

and the coupling matrices are given by

$$A_{\alpha\beta}(x) = \int \phi^*_\alpha(y;x)\partial_x\phi_\beta(y;x)dy, \tag{5}$$

$$B_{\alpha\beta}(x) = \int \phi^*_\alpha(y;x)\partial^2_x\phi_\beta(y;x)dy. \tag{6}$$

What we shall call the *global* adiabatic approximation consists in neglecting the right hand side of Eq. (3) completely. As a result, the equations decouple into one-dimensional Schrödinger equations for the various modes, with the transverse eigenvalue $E_\alpha(x)$ acting as an effective barrier potential. With hard wall confinement, these effective barriers will be inversely proportional to the width square, $E_\alpha(x) \sim W^{-2}(x)$. With parabolic confinement, $E_\alpha(x) \sim W^{-1}(x)$. As a consequence, for given $W(x)$, a constriction with hard walls will appear as more abrupt than one with parabolic confinement. Note that there are speculations in the literature[10] that the global adiabatic approximation might be *exact* for a single QPC, as far as its conductance is concerned.

An apparent improvement over the global adiabatic approximation consists in retaining the diagonal terms on the right hand side of Eq. (3), while again discarding all nondiagonal ones. This is what we call the *diagonal* approximation (called adiabatic by several authors), and again results in a set of one-dimensional effective barrier problems. The extra terms retained stem from $B_{\alpha\alpha}$ and produce an additional contribution to the effective barriers, proportional to $(W'/W)^2$. Castaño and Kirczenow[9] have shown that when stepwise behavior breaks down according to the diagonal approximation (which they call adiabatic), exact calculations still give a stepwise conductance.

III. RESULTS

A. Comparisons

In order to compare, with some flexibility, the three approximations of the preceding section with exact results, we use QPC's with somewhat different shapes. At

this point we limit ourselves to constrictions with fourfold symmetry (mirror symmetry around $x = 0$ and $y = 0$) to keep comparisons as simple as possible. For $|x| > L$, let the width of our infinite waveguide be W_∞. This is also chosen to be the maximum width. The total length of the symmetric constriction is $2L$, and the minimum width W_0. We use the following two shapes:

$$\frac{W_1(x)}{W_\infty} = \begin{cases} \frac{W_0}{(W_\infty - W_0)\cos^4(\pi x/2L) + W_0}, & |x| \le L \\ 1, & |x| > L \end{cases} \quad (7)$$

$$\frac{W_2(x)}{W_\infty} = \begin{cases} 1 - \left(1 - \frac{W_0}{W_\infty}\right)\cos^2\left[\frac{\pi}{2}\left(\frac{x}{L}\right)^P\right], & |x| \le L \\ 1, & |x| > L. \end{cases} \quad (8)$$

Shape 1 is the one considered in Ref. 9. With $P = 1$, shape 2 corresponds to that of Ref. 10.

Results for the conductance in units of $2e^2/h$ as a function of $k_F W_0/\pi$ (i.e., of the square root of the dimensionless energy) are presented in Fig. 1. We have used hard wall boundaries, shape 1 in Fig. 1(a), shape 2 with $P = 1$ in Fig. 1(b), and have chosen ratios such that $W_\infty/W_0 = 6$ and $L/W_0 = 1$ in both cases. The most striking feature of Fig. 1 is the failure of the diagonal approximation, found already by Castaño and Kirczenow[9] for precisely the QPC of Fig. 1(a). As explained in Ref. 9, the artificial resonances of the diagonal approximation are due to the "ears" contributed to the effective barrier potentials by $B_{\alpha\alpha}(x) \sim (W'/W)^2$. For constrictions of increasing abruptness, these artificial resonances become progressively more prominent. However, the global adiabatic approximation, which neglects $B_{\alpha\alpha}$ along with all the coupling terms, is more successful. In fact, it is remarkably successful, considering the abruptness of the constrictions shown. In particular, this approximation does not produce *qualitatively* wrong results for the conductance of a single QPC. This highlights the inconsistency of the diagonal approximation: One should not keep diagonal terms on the right hand side of Eq. (3), while neglecting equally important nondiagonal ones. Quantitatively, however, even the results based on the global adiabatic approximation show clear deviations from the exact results, contradicting the speculations in Ref. 10. The *local* adiabatic approximation fares worse, and essentially washes out the conductance steps, in spite of the fact that the smoothness parameter κ of Eq. (2) takes the values 4.87 and 2.81, respectively, for the two shapes of Fig. 1.

Note that the above comparisons between numerically exact and approximate methods were based on the results for the conductance alone. It is important to distinguish between the fundamental merits of the global approximation itself, which neglects intermode scattering altogether, and its qualities as a method for calculating the conductance. With the abrupt constrictions of Fig. 1, it is not surprising that intermode scattering is considerable. However, as emphasized by Brataas and Chao,[10] in spite of this, the conductance predicted by the global adiabatic approximation can be extremely close to the exact one. Reasons for this have been pointed out by Yacoby and Imry.[8] In their careful discussion[11] of the leading corrections to the adiabatic approximation they show that, whereas the local transmission amplitudes $|t_{\alpha\beta}(x)|$ scale with $W'(x)N_{av}(x) = W'(x)W(x)k_F/\pi$, where $N_{av}(x)$ is the locally available number of propagating modes, the corresponding reflection amplitudes scale with $W'(x)/N_{av}(x)$. With constrictions that allow essentially adiabatic transport in the inner region, with only N_0 modes propagating in the narrowest part, these scaling relations explain the strongly reduced backscattering where the constriction rapidly opens up, and $N_{av} > N_0$. Even when the nondiagonal terms of the transmission matrix are appreciable, the deviations in the conductance

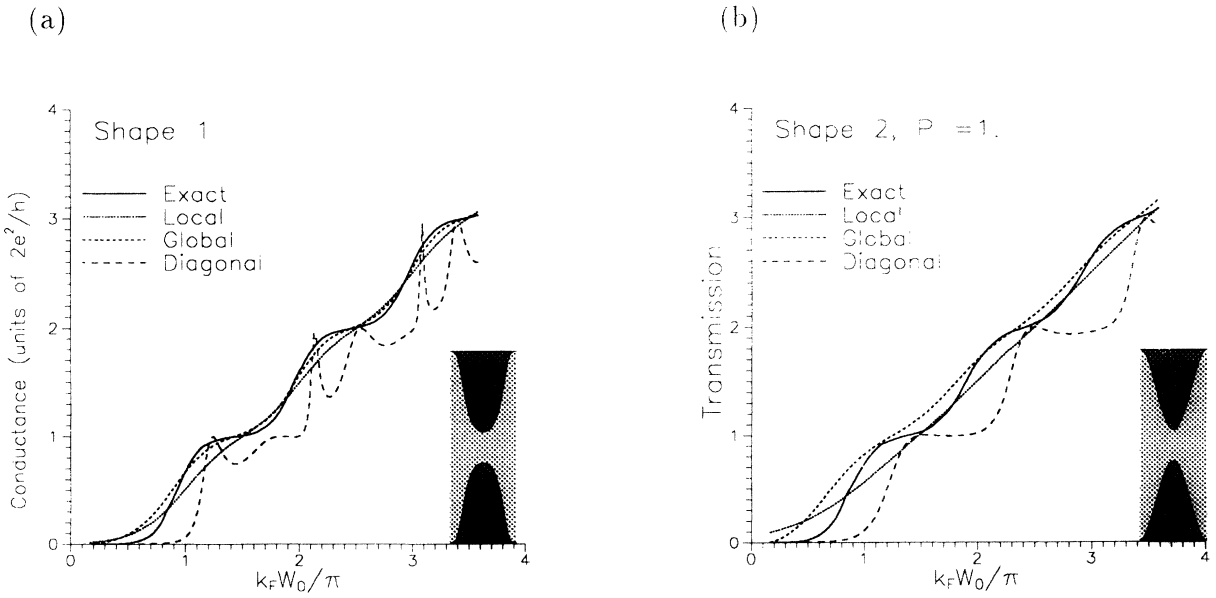

FIG. 1. The conductance as a function of the Fermi wave number for two QPC's of different shape, both with $W_\infty/W_0 = 6$ and $L/W_0 = 1$. In both cases "exact" numerical results (full line) are compared with three popular approximations.

from its adiabatic value, determined essentially by the reflection amplitudes, can be small.

In spite of the success of the global adiabatic approximation in predicting the conductance of a single QPC (with more examples to be given below), deviations from the exact results can, under certain circumstances, be clearly seen. Refinements of the physical picture are then called for.

B. A qualitative picture

An interesting fact demonstrated by Fig. 1 is the more pronounced stepwise behavior of the conductance in the exact calculations than in those based on the global adiabatic approximation. We shall now argue that this is no accident, but has a simple physical explanation. The argument that follows must only be read as a qualitative guide, applicable under certain (realistic) circumstances.

For easier understanding, first consider a geometry (with hard wall boundaries) where the width of the quantum wire abruptly jumps from W_∞ to W_0 ($W_\infty \gg W_0$) and, after a length $2L$, jumps back to W_∞. This extreme case was discussed already in 1989 by Szafer and Stone.[12] They showed, by simple Fourier analysis, that the propagating mode with transverse wave number q_n in the constriction is mostly fed by incoming modes with transverse wave numbers close to q_n. In fact, the uncertainty relation immediately gives that $\Delta q \sim W_0^{-1}$. Similarly, this mode (propagating or evanescent) will produce a superposition of outgoing modes with the same distribution over transverse wave numbers. Since the total energy E is conserved, a width Δq in the distribution of transverse wave numbers will produce a corresponding distribution of *longitudinal* wave numbers centered around k_n (or around κ_n if the mode is evanescent, and κ_n is the corresponding damping coefficient). Here $2m^*E/\hbar^2 \equiv k_F^2 = q_n^2 + k_n^2$ (or $k_F^2 = q_n^2 - \kappa_n^2$). With k_n (or κ_n) close to the threshold, where $k_n = \kappa_n = 0$, this distribution will typically be over propagating modes (width Δk), as well as evanescent ones (width $\Delta\kappa$). The order of magnitude will be the same, $\Delta k \sim \Delta\kappa \sim \Delta q \sim W_0^{-1}$. In contrast to the uncorrelated modes impinging on the constriction, outgoing modes originating in a single constriction mode have rigid phase relations. As a consequence, a spread in longitudinal wave numbers corresponds to a persistence length in the wave pattern emerging from the constriction. In other words, *the effective length of the constriction is longer than the geometric length*, near threshold by roughly the amount

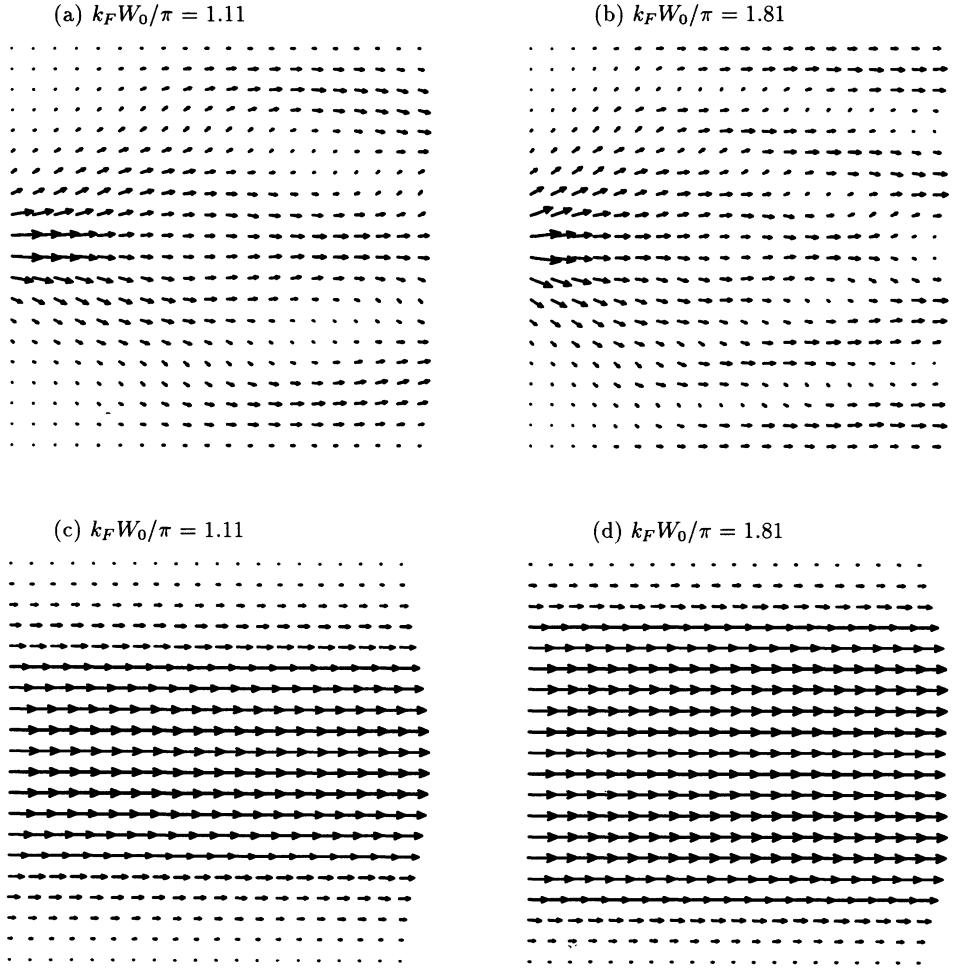

FIG. 2. Current density plots for the QPC of Fig. 1(b). Scaling of the arrows is arbitrary for each plot. Plots (a) and (b) show current densities according to exact calculations, whereas (c) and (d) are calculated according to the global adiabatic approximation. The current densities are shown on the x interval $(L, L + W_\infty)$, where $x = L$ can be regarded as the exit of the constriction. The numerical values for k_F, given at the top, show that (a) and (c) correspond to a Fermi energy slightly higher than the threshold for propagation of mode 1, whereas for (b) and (d), the energy is approaching the threshold for mode 2.

$l \sim [\max(\kappa_n, \Delta k, \Delta\kappa)]^{-1} \sim W_0$.

This argument was based on the simplest possible geometry with sudden jumps in the width of the electron waveguide, for which the global adiabatic approximation, strictly speaking, has no meaning. As a qualitative guide the argument also applies to QPC's with smooth geometries and sufficiently rapidly varying widths, like those of Fig. 1, that the current density is unable to follow the rapid change in geometry. For such geometries the global adiabatic approximation *is* well defined. As a rough estimate, our calculations indicate that $W'(x)$ must be considerably greater than unity for the effect to exist, i.e., for the persistence length to be meaningful. All this is demonstrated in Figs. 2(a) and 2(b), which show, for two different energies on the first conductance step, the current density emanating from the exit (defined as $x = L$) of the QPC of shape 2 [see Fig. 1(b)]. For comparison, the corresponding current densities, as given by the (in this context obviously unreliable) global adiabatic approximation, are shown in Figs. 2(c) and 2(d). The effective lengthening l of the constriction is clearly of the same order as W_0. Furthermore, one can see that when the energy is close to the threshold, $\max(\kappa_n, \Delta k, \Delta\kappa)$ is at its minimum. One would therefore expect that the effective length of the constriction is somewhat greater here. This can be recognized in the slightly longer persistence length of Fig. 2(a) than of Fig. 2(b).

Three remarks are in order. (i) From time reflection invariance (no magnetic field here) the effects seen at the far end of the constriction must have precise counterparts at the entrance. However, in the current density these effects, at the entrance, can be masked by totally reflected modes. (ii) In addition to increasing the effective length of the constriction, the mechanism described above also effectively smoothens the shape of the constriction (in both ends), so as to reduce the probability for reflections. (iii) In a sense, the mechanism under discussion plays a role complementary to that of collimation.[13,14] Collimation is seen in constrictions with slowly increasing width, so that adiabaticity leads to a transfer of energy from the transverse to the longitudinal direction. The present mechanism, in contrast, takes over when the widening has become so rapid that adiabaticity breaks down, and no further energy transfer (on average) takes place.

One direct consequence of the effective lengthening of the constriction is the sharpening of the conductance steps of QPC's, as compared with the results of the global (not to mention the local) adiabatic approximation. This is demonstrated already in the results shown in Fig. 1. A further consequence of the mechanism discussed will become apparent in Fig. 4 below.

C. A realistic QPC

Encouraged by the success of our numerical scheme, we now turn to calculations on a QPC with a geometry close to that used in the experiments by van Wees *et al.*[1,15] After their initial report on quantization with this type of QPC, a theoretical calculation was performed on a similar structure by Tekman and Ciraci.[16] Their results for QPC's with sharp corners, similar to real QPC's as defined lithographically, showed poor quantization. This led van Wees *et al.*[15] to conclude that the actual electrostatic potential that defines the QPC's is substantially different from the geometry of the lithographic gate. Self-consistent, and smooth, electrostatic potentials have been calculated by Kumar *et al.*[17] and by Nixon *et al.*[18] It is therefore of interest to see how far from the sharp gate geometry one needs to go before quantization of the conductance is achieved. We model the geometry of the QPC by the following analytic form (shape 3):

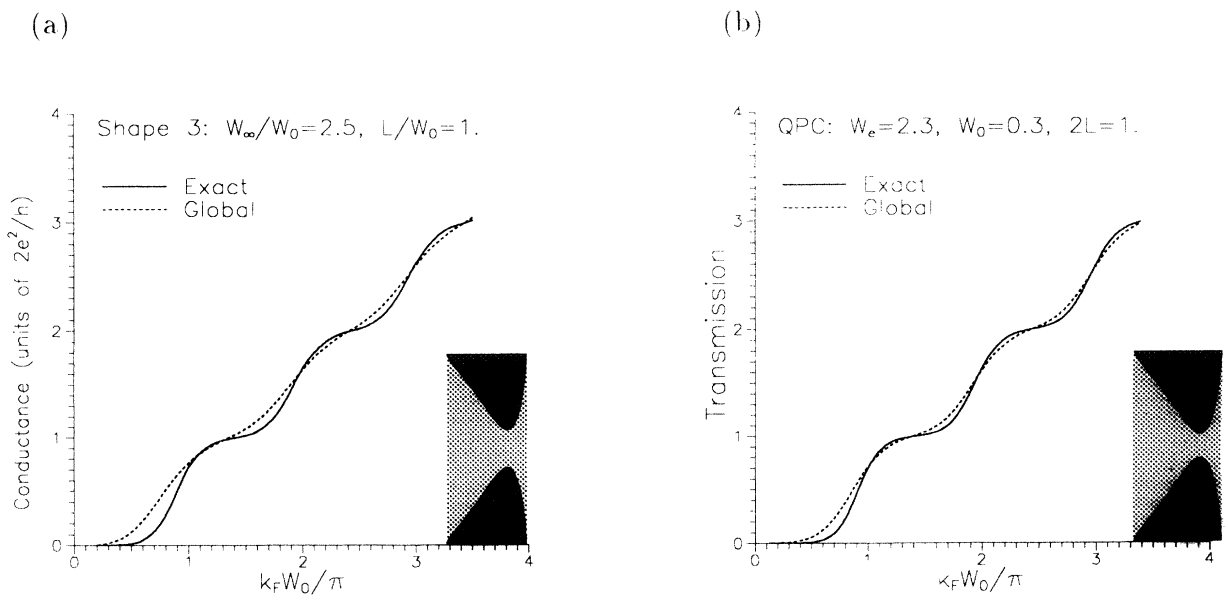

FIG. 3. The conductance of QPC's with realistic shapes, shown in the insets. In (a) $W_\infty/W_0 = 5$ and $L/W_0 = 1$. In (b) $W_\infty/W_0 = 23/3$ and $L/W_0 = 5/3$.

$$\frac{W_3(x)}{W_\infty} = \begin{cases} 1 - \left(1 - \frac{W_0}{W_\infty}\right) \cos^\gamma[f(x/L;Q)], & |x| \le L \\ 1, & |x| > L \end{cases}$$

$$f(u;Q) = \frac{\pi}{2\sinh Q}[\exp(Qu) - \cosh Q]. \quad (9)$$

The resulting geometry is shown in Fig. 3 for $\gamma = 0.7$ and $Q = 1.3$. Figure 3(a) shows the case when $W_\infty/W_0 = 5$ and $L/W_0 = 1$, whereas in Fig. 3(b) $W_\infty/W_0 = (23/3)$ and $L/W_0 = 5/3$. The latter gives a slightly better quantization of the conductance. This can be understood in terms of the smoothness parameter, $\kappa = \pi^2\sqrt{2R/W_0}$, which is larger in case (b), due to the smaller W_0. The geometry of Fig. 3(b) is probably the one closest to the real device. Our results show that for both cases, exact calculations give good quantization, whereas the steps are considerably more smeared out according to the global adiabatic approximation.

D. Resonance effects in QPC's

A number of calculations on QPC's show resonant behavior in the conductance, due to backscattering at the exit and the entrance of the constriction.[12,16,19] The relevance of these calculations has been questioned[15,20] since they use unrealistic constriction geometries with sharp corners that greatly enhance the probability for reflection. With our powerful numerical scheme, we are in a position to check the extent to which resonances occur in smoothly varying geometries. We have considered two cases.

First, we consider QPC's with a finite region (length L_0) of constant width W_0 in the middle. The two connecting regions, each of length ΔL, are of shape 2, as defined by Eq. (8), with $L \to \Delta L$ and with $P = 2$. With $W_\infty/W_0 = 6$ and small connection lengths, $\Delta L/W_0 = 3/8$, as used in Fig. 4(a), oscillations are prominent. For completeness, we have again included the diagonal approximation, which is clearly misleading here. Both the global adiabatic approximation and the exact calculations yield pronounced oscillations. It is interesting to note that the oscillations of the exact results have higher frequencies and lower amplitudes than those of the global adiabatic approximation. This can be understood on the basis of the qualitative picture given in Sec. III B. The increase of the effective length of the constriction, not seen in the global adiabatic approximation, is responsible for the higher frequency of the exact oscillations. Similarly, the effectively smoothened connections between the constriction and the external 2DEG reduce the reflection probabilities, with smaller oscillation amplitudes as a result. We have tested this interpretation by calculating the conductance with the same parameters as in Fig. 5(a), except that L_0 is increased by a factor 3. As expected, the frequencies of the oscillations according to the exact and adiabatic results are now much closer to one another, whereas the ratio of their amplitudes is essentially unaffected.

The much longer connection length, $\Delta L/W_0 = 5$, used in Fig. 4(b), dampens the oscillations considerably. In agreement with our qualitative picture [$W'(x) \lesssim 1$ here], the difference between the global adiabatic approximation and the exact results for the conductance is hardly noticeable with such smooth connections, in spite of the fact that mode mixing is considerable. It is more surprising that oscillations are at all present in this case.

Against the case studied above, one could argue that

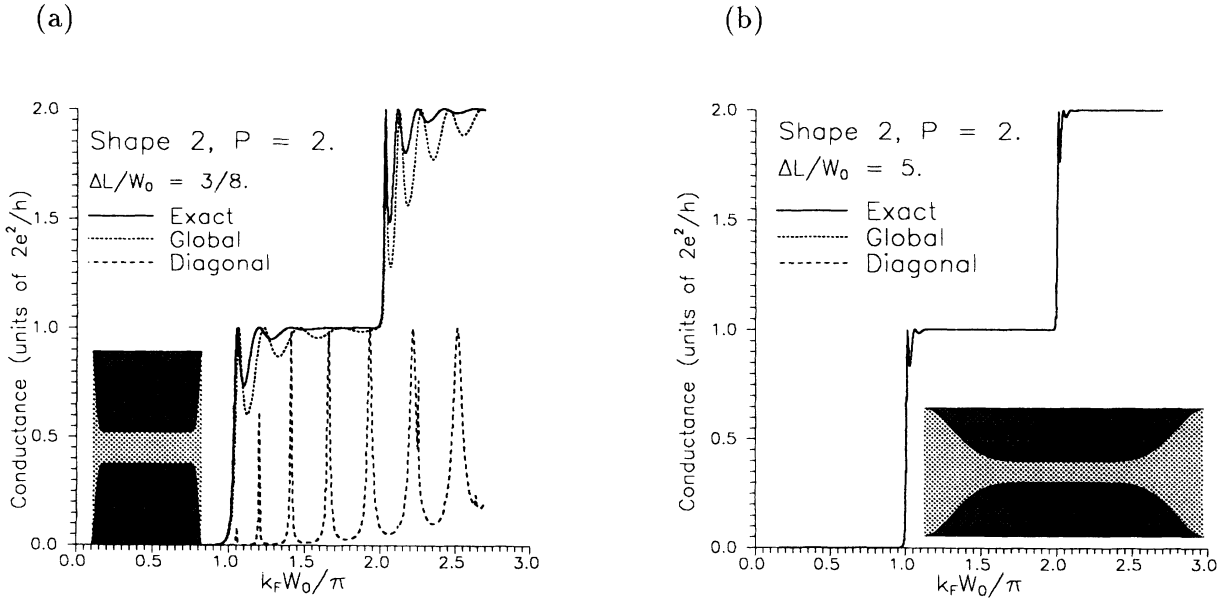

FIG. 4. Resonance effects in QPC's. The figure shows the conductance of two QPC's according to exact results and calculations based on the global adiabatic and diagonal approximations. Both QPC's have an inner region of constant width W_0 of length L_0, with $L/W_0 = 5/2$, and a ratio $W_\infty/W_0 = 6$. In (a) the connection regions are short, with $\Delta L/W_0 = 3/8$. In (b) the connection regions are considerably longer, with $\Delta L/W_0 = 5$.

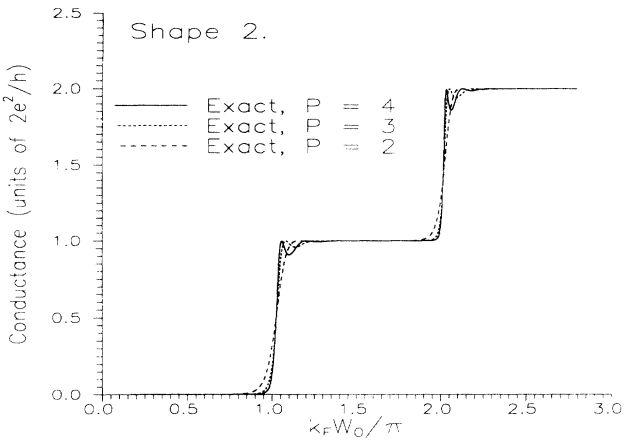

FIG. 5. Resonance effects in QPC's. The figure shows the conductance for three QPC's with different shapes, all of them continuous. For all three constrictions, $W_\infty/W_0 = 6$ and $L/W_0 = 5/2$. The maximum of $W'(x)$ increases with increasing P, thereby enhancing the probability for reflection.

QPC's with entirely straight segments are unrealistic and, furthermore, that this model forces the second derivative of $W(x)$ to jump at the ends of the straight segment, even though the first derivative is continuous. As our second case we have therefore also looked for resonances in QPC's with completely continuous geometries. Figure 5 shows exact results for QPC's of shape 2, given by Eq. (8) (with no straight part inserted), for three different values of the exponent P. We have chosen parameters such that $W_\infty/W_0 = 6$ and $L/W_0 = 2.5$. Whereas no oscillations occur for $P = 2$, they are clearly visible, if not exactly prominent, for $P = 3$ and $P = 4$. This demonstrates that resonances can indeed result from rapidly changing, but completely continuous geometries. Whether experimentally observed resonances should be explained by this mechanism is quite another matter. Impurity scattering is a more likely candidate.

IV. CONCLUDING REMARKS

In this paper we have studied the influence of geometry on linear transport through QPC's. By combining two standard techniques in the field, we constructed a numerical scheme sufficiently powerful and flexible that approximations commonly used could be tested against "exact" numerical results for a number of QPC geometries. Our calculations confirm[9] that the diagonal approximation can produce a qualitatively wrong result and is, therefore, not to be trusted. The local adiabatic approximation[6] is of limited value as a basis for explaining the observed conductance steps in single QPC's. However, the *global* adiabatic approximation is remarkably good in its predictions of the conductance of a single QPC. Nevertheless, even for single QPC's, with sufficiently rapidly changing width, this approximation underestimates the sharpness of conductance steps. The reason for this has been pinpointed: The coupling between inner and outer modes leads to constrictions that are effectively longer and smoother than given by their geometry alone. The result is a sharpening of the conductance steps. The most convincing evidence for the correctness of this qualitative picture is provided by the frequency and amplitude of the oscillations shown in Fig. 4(a).

Even though the global adiabatic approximation in many cases correctly predicts the conductance of single QPC's, its basic flaw, associated with the neglect of all intermode scattering, becomes apparent in more complex situations. The simplest example is transport through two QPC's in series. With intermode scattering neglected, the adiabatic approximation predicts negligible reflection by the second QPC, once the first one has been passed. In reality, intermode scattering leads to substantial reflection, also by the second QPC. For similar reasons, the adiabatic approximation fails in the presence of impurities, as convincingly demonstrated by Nixon *et al.* and Laughton *et al.*[18,21] With impurities, both intermode scattering and a correct treatment of phase relationships are essential for a realistic calculation of the conductance (with or without resonances). All these comments apply to the case of zero (or weak) magnetic field. Glazman and Jonson[22] have shown how the global adiabatic approximation becomes valid, in the sense that mode mixing becomes negligible, in sufficiently strong fields. Temperature effects will smear out oscillations both in exact and adiabatic calculations, and the experimentally observed simple steps in the conductance of QPC is presumably partly due to temperature smearing of fine oscillatory details.

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APPENDIX A

The transverse continuum Schrödinger equation was given in (4). We now discretize the x axis, $x_m = ma$, with a the lattice constant, and write the total wave function in ket notation,

$$\Psi(x_m, y) = \sum_\alpha \chi_\alpha(x_m)|\alpha, m\rangle. \tag{A1}$$

To each point m on the x chain is associated the energy eigenstate $\alpha = 1, 2, 3, \ldots$. The Hamiltonian, of the tight binding type, acting on the states of this chain reads

$$H_{\mathrm{TB}} = \sum_{\alpha,m} |\alpha, m\rangle(\epsilon_m^\alpha + 2)\langle\alpha, m| - \sum_{\alpha,\beta,m} \left[t_{m,m+1}^{\alpha\beta} |\alpha, m\rangle\langle\beta, m+1| + t_{m+1,m}^{\alpha\beta} |\alpha, m+1\rangle\langle\beta, m| \right], \tag{A2}$$

with

$$\epsilon_m^\alpha = \frac{2m^*a^2}{\hbar^2} E_\alpha(x_m) \tag{A3}$$

and

$$t_{m,m+1}^{\alpha\beta} = \int \phi_\alpha^*(y;x_m)\phi_\beta(y;x_{m+1})dy. \tag{A4}$$

The corresponding Schrödinger equation is

$$H_{TB}\Psi = \epsilon\Psi, \tag{A5}$$

with $\epsilon = (2m^*a^2/\hbar^2)E$. It is straightforward to check, by Taylor expansion to second order in a, that (A5) in the continuum limit, $a \to 0$, reduces to the set of equations (3)–(6). Note that the tight binding Hamiltonian (A2) has only nearest neighbor couplings in the x direction. In the energy "direction," however, all "sites" α are, in principle, coupled to all "sites" β on the neighboring x slice, according to (A4). Symmetry can, of course, reduce the number of nonzero couplings.

In principle, the number of transverse eigenstates is infinite. However, for a realistic Fermi energy, a numerical scheme based on truncation after a few modes beyond the M_p modes propagating in the widest part of the given structure rapidly converges. Typically, depending on the circumstances, one needs to include no more than five evanescent modes. This means that for many problems of interest, one has $M \lesssim 20$, and the dimension, $M \times M$, of matrices to be repeatedly inverted is easily handled, when transport along the x chain is calculated by the recursive Green function technique.[5] A *direct* application of this technique to the discretized xy plane requires much larger matrices. The price one has to pay in this context, using our hybrid method, is associated with the fact that $t_{m,m+1}^{\alpha\beta}$ couple "all" states, α. This price is essentially negligible.

Generalization to the case with nonzero magnetic field is immediate, accomplished by using the Peierls substitution when the overlap integrals (A4) are calculated.

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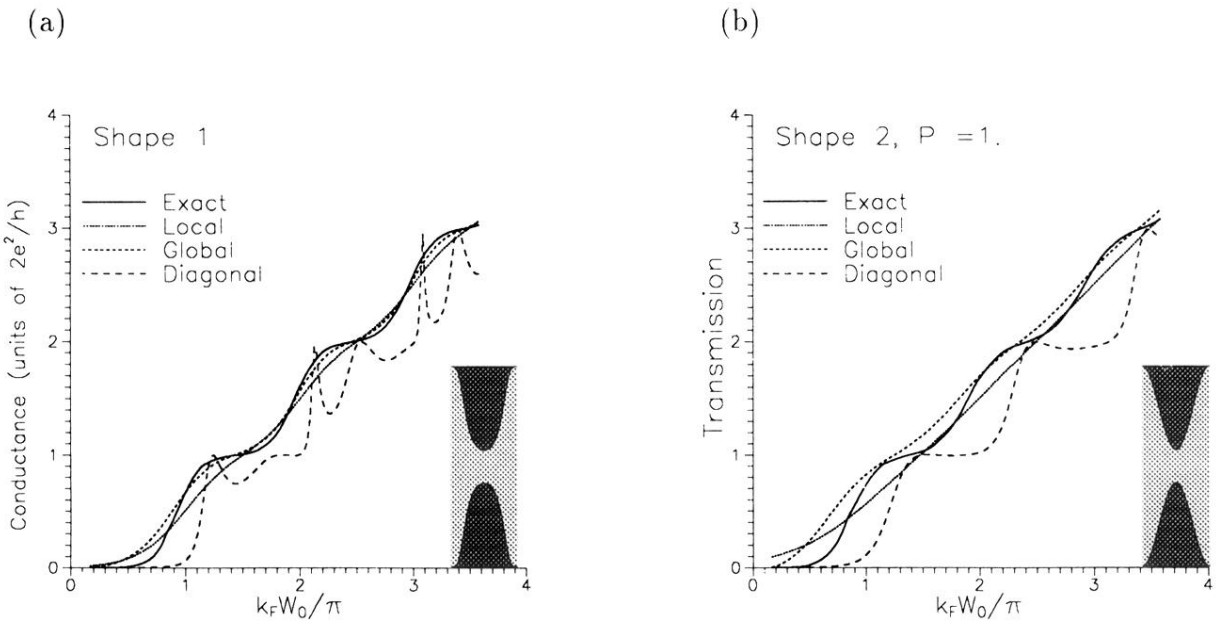

FIG. 1. The conductance as a function of the Fermi wave number for two QPC's of different shape, both with $W_\infty/W_0 = 6$ and $L/W_0 = 1$. In both cases "exact" numerical results (full line) are compared with three popular approximations.

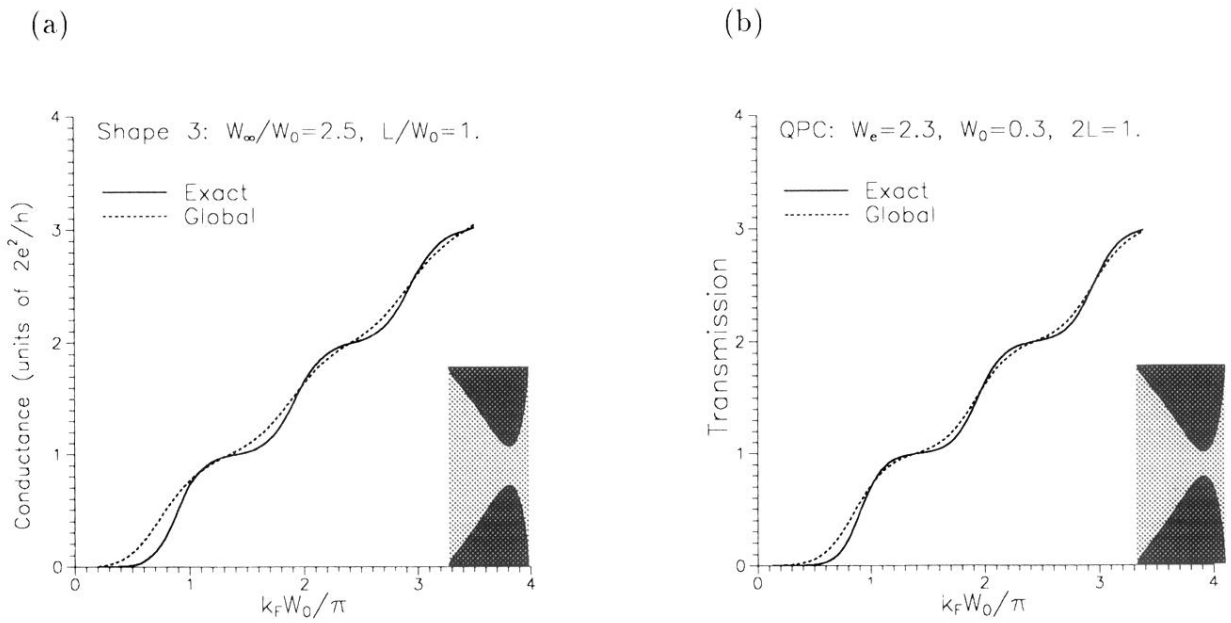

FIG. 3. The conductance of QPC's with realistic shapes, shown in the insets. In (a) $W_\infty/W_0 = 5$ and $L/W_0 = 1$. In (b) $W_\infty/W_0 = 23/3$ and $L/W_0 = 5/3$.

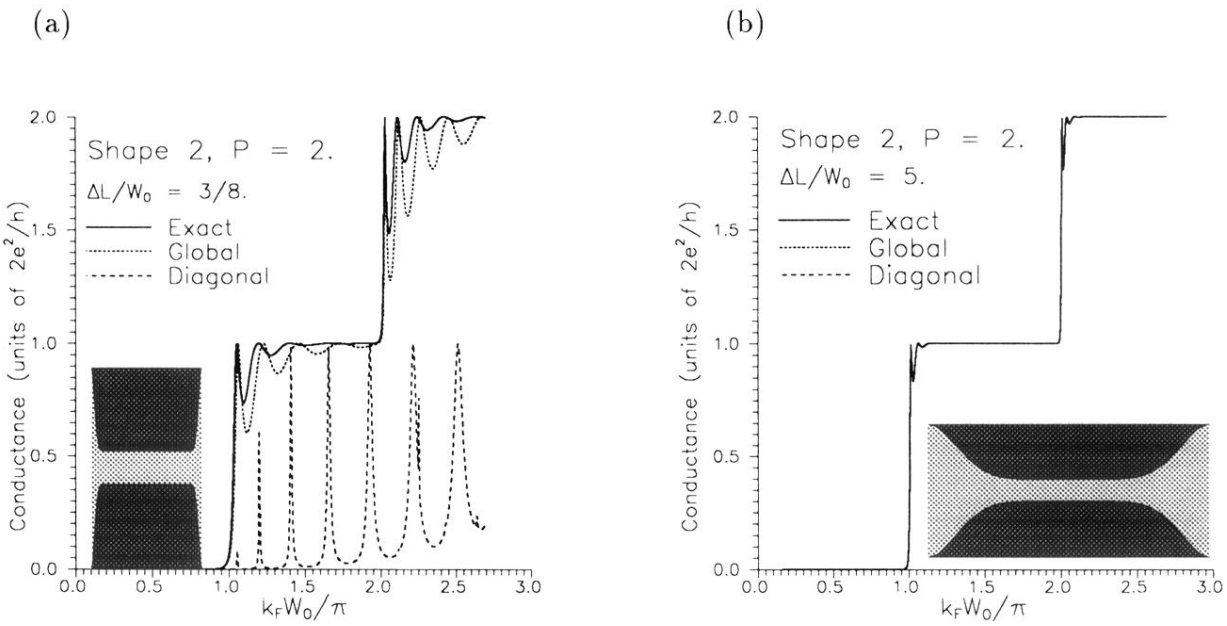

FIG. 4. Resonance effects in QPC's. The figure shows the conductance of two QPC's according to exact results and calculations based on the global adiabatic and diagonal approximations. Both QPC's have an inner region of constant width W_0 of length L_0, with $L/W_0 = 5/2$, and a ratio $W_\infty/W_0 = 6$. In (a) the connection regions are short, with $\Delta L/W_0 = 3/8$. In (b) the connection regions are considerably longer, with $\Delta L/W_0 = 5$.