Modal analysis of transport through quantum point contacts using realistic potentials

Michael J. Laughton, John R. Barker, John A. Nixon,* and John H. Davies†
Department of Electronics and Electrical Engineering, University of Glasgow, Glasgow G12 8QQ United Kingdom
(Received 18 January 1991)

We have studied conduction through quantum point contacts using a coupled-mode analysis and realistic potentials. Disorder causes transport to be strongly nonadiabatic with rapid intermode scattering. The conductance can remain well quantized because of the predominantly forward nature of the scattering. Resonances in the channel lead to strong *indirect* backscattering that cannot be described by the Born approximation. This degrades quantization in point contacts and reduces the mobility of narrow wires.

The observation of the quantized conductance of a narrow constriction or "quantum point contact" formed in a two-dimensional electron gas [1,2](2DEG) stimulated a rapid growth in the study of electron transport in quasi-one-dimensional systems.[3] Much of the modeling of such devices has used the recursive Green's-function technique.[4] This is a powerful method but gives little direct insight. The quantization of electrons into transverse modes leads naturally to an analogy with electromagnetic waveguides, and transport can be viewed in terms of the local transverse modes. This gives a much more physical picture, and has been extensively used near the adiabatic limit where intermode scattering is weak.[5] However, recent numerical calculations[6] have shown that the ionized donors in a heterostructure make an important random contribution to the potential in electron waveguides. The nature of transport in such potentials is expected to be nonadiabatic.[7] It is important to gain a physical insight into the scattering mechanisms of real quasi-one-dimensional structures.

We have analyzed electron transport in realistic models of point contacts in terms of local transverse modes without making the adiabatic approximation: the full intermode coupling is retained. Our model includes the guiding potential from patterned gates and the random potential from ionized donors. We find that the random contribution to the potential makes transport strongly nonadiabatic, even in samples that show well-quantized conductance. Scattering is predominantly forward because the random potential is slowly varying: an electron changes mode but keeps going in the same direction, preserving the conductance. A major cause of poor quantization is *indirect* backscattering that occurs through resonances trapped in bulges in the channel.

For the modal analysis, take coordinates so that current flows along x, with transverse confinement in y. At each value of x, solve the transverse Schrödinger equation in y to find the eigenfunctions $\theta_n(y;x)$ and energies $\varepsilon_n(x)$. The dependence on x arises because the transverse potential varies along the length of the structure. The full wave function at energy E is then expanded in terms of these transverse eigenfunctions (modes),

$$\Psi(x,y)=\sum_n \{c_n^+(x)\exp[ik_n(x)x] + c_n^-(x)\exp[-ik_n(x)x]\}\phi_n(y;x)\,, \tag{1}$$

where $c_n^{\pm}(x)$ is the amplitude of the electrons traveling forwards (+) or backwards (−) in the n^{th} transverse mode. The propagation constants

$$k_n(x)=\sqrt{2m[E-\varepsilon_n(x)]/\hbar^2}$$

may be real or imaginary, corresponding to propagating or evanescent modes. A transverse mode energy $\varepsilon_n(x)$ increases when the point contact narrows, and may reach a point where $\varepsilon_n(x)=E$. At this point $k_n(x)$ falls to zero, the mode is cut off, and the electron is reflected unless it can tunnel through the narrow region. There are $n_m(x)$ propagating modes at each cross section, of which $n_{\min}$ are "conducting" modes that are never cut off and propagate through the whole system.

We have developed a method for determining the modal occupancy in a numerically stable and efficient manner.[8] Substituting Eq. (1) and the potential profile into the two-dimensional Schrödinger equation leads to a coupling between the transverse modes that is omitted from the adiabatic approximation. The resulting equations form a two-point boundary-value problem with each mode contributing two equations. The two exponential growth classes of the solution can be integrated without numerical instability to provide the amplitudes $c_n^{\pm}(x)$ throughout the system. The results are expressed in terms of t and r matrices, defined as usual for propagating modes by

$$t_{kj}(x)=\left[\frac{k_k(x)}{k_j(x=0)}\right]^{1/2}\frac{c_k^+(x)}{c_j^+(x=0)} \tag{2}$$

and

$$r_{kj}(x)=\left[\frac{k_k(x)}{k_j(x=0)}\right]^{1/2}\frac{c_k^-(x)}{c_j^+(x=0)}\,, \tag{3}$$

where $x=0$ is the left-hand edge of the system. Then $|t_{kj}(x)|^2$ is the probability that flux input in mode j is traveling forward in mode k at x, and similarly $|r_{kj}(x)|^2$ is the probability that flux input in mode j is traveling backward in mode k at x. The dimensionless conductance [in units of $(2e^2/h)$] is given in terms of the overall t matrix by $G=\mathrm{Tr}(t^\dagger t)$. The t matrix reduces to the identity in an adiabatic system, and there is perfect quantization with $G=n_{\min}$.

We have applied this method to transport through the central regions of quantum point contacts defined by split gates, using realistic potentials. These potentials were determined self-consistently by Nixon, Davies, and Baranger[7] using a semiclassical Thomas-Fermi approximation. They include the ionized donors in the n-doped layer of the heterostructure, which produce a random potential with long-ranged fluctuations that deform the smooth potential from the gate alone. Parameters of the structure were taken from Timp *et al.*[9] The gates are 600 nm long with a 300-nm gap between them; we modeled these long point contacts so that we could distinguish events within the channel from those at the entrance and exit. Ten modes are retained throughout the calculation, whether they are propagating or evanescent. Ideal leads are attached to the system by extending the potential profile at the left and right edges out to infinity. Our conductances agree within a few percent with those of Nixon, Davies, and Baranger,[7] who used the recursive Green's-function method.

A well-quantized device with $G=1$ [curve B in Fig. 2(b) of Ref. 7] is illustrated in Fig. 1. The density of electrons shows fluctuations caused by the random potential. The number of propagating modes $n_m(x)$ in Fig. 1(b) has a minimum $n_{\min}=1$, consistent with the conductance. To study the transport we define

$$a_k^+(x)=\sum_j |t_{kj}(x)|^2 , \quad a_k^-(x)=\sum_j |r_{kj}(x)|^2 . \tag{4}$$

Then $a_k^\pm(x)$ is the probability of occupancy of the forward (+) or backward (−) mode k at x along the constriction, irrespective of the mode in which the electron entered the system. If transport were adiabatic, each $a_k^+(x)$ would remain unity until cutoff at which point its flux would be entirely reflected into $a_k^-(x)$. At first sight, Fig. 1(b) for the forward occupancy $a_k^+(x)$ appears to support this. However, there is forward scattering after the narrowest part of the point contact, when higher modes become available. The occupancies of the backward-going modes $a_k^-(x)$, shown in Fig. 1(c), are also inconsistent with the adiabatic approximation. In particular there is substantial occupation of the lowest mode, which should be empty.

To study the scattering further, we have analyzed the flux in terms of the modes in which the electrons *entered* the sample [Figs. 1(d) and 1(e)]. Define

$$b_j^+(x)=\sum_k \left|t_{kj}(x)\right|^2 , \quad b_j^-(x)=\sum_k \left|r_{kj}(x)\right|^2 , \tag{5}$$

so that $b_j^\pm(x)$ is the probability that flux input in mode j is traveling forward (+) or backward (−) at x, irrespective of which mode it is in at x. Thus $b_j^\pm(x)$ resolves the flux into *input* modes, whereas $a_n^\pm(x)$ resolves the flux

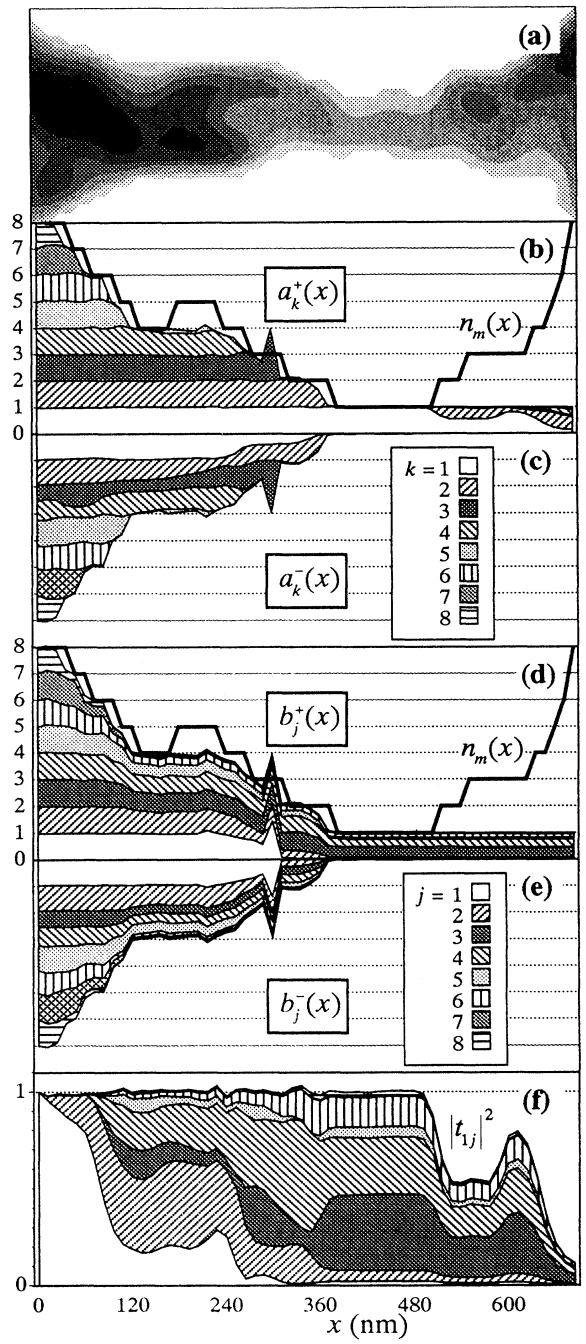

FIG. 1. Point contact with well-quantized conductance $G=1$. (a) Electron density with 4.2×10^{14} m^{-2} between levels of gray; (b) forward and (c) backward flux resolved into modes at x; (d) forward and (e) backward flux resolved into input modes; (f) origins of flux in the lowest mode. The number of propagating modes at each cross section, $n_i(x)$, is superposed on (b) and (d).

into *local* modes at x. The absence of scattering in the adiabatic limit implies $b_n^{\pm}(x)=a_n^{\pm}(x)$. This is clearly not the case. In particular, electrons the enter in the lowest mode make a tiny ($\approx 2\%$) contribution to the conductance. The origins of the flux in this mode, the only conducting mode in this system, are shown in Fig. 1(f). Most electrons that enter the sample in this mode are rapidly scattered out, but are replaced by electrons that entered in higher modes so that the total flux remains unity. The fractions contributed by the different incident modes remain constant only in the narrowest region of the constriction, where $n_m(x)=n_{\min}$. This is the sole region where transport can be said to be adiabatic. Even this is not true in a wider constriction with $n_{\min}>1$, where we have found scattering between the conducting modes in other well-quantized samples. In contrast, we have also studied a smooth potential with no randomness. In this case the adiabatic approximation held to within a few percent.

The results in Fig. 1 show that it is possible to have well-quantized conductance even when scattering is strong and the adiabatic approximation fails. Two conditions must be met for quantization: the conducting modes must be fully occupied when they reach the narrowest part of the constriction, and they must not be backscattered after this point. These conditions are fulfilled in our system because forward scattering is dominant, which in turn follows from the slowly varying nature of the random potential in space. Forward scattering allows a "compensating" process to occur to the left of the constriction. Figure 1(b) shows that all the forward-going modes are fully occupied until they reach cutoff. Electrons that scatter out of one of the conducting modes into a higher mode can therefore be exactly balanced by electrons scattering via the inverse process. This would not be true if backscattering were important, because the backward-going modes are not fully occupied and the two rates would not balance. Compensation was suggested by Payne,[10] who studied a channel whose width changed with time. Pure forward scattering is also analogous to a unitary change of basis, under which $\mathrm{Tr}(t^{\dagger}t)$ is invariant.[11]

We have also studied a poor device to investigate the breakdown of quantization. Figure 2 shows transport through a point contact which is identical to that of Fig. 1 except for a different random distribution of ionized impurities [curve C in Fig. 2(b) of Ref. 7]. A slight change in gate voltage from $V_g=-0.724$ V (Figs. 2(b) and 2(c)] to -0.720 V [Figs. 2(d) and 2(e)] leads to a *decrease* in conductance from $G=1.71$ to $G=1.55$, whereas an *increase* would have been expected as the channel becomes wider and deeper. The electron density and $n_m(x)$ show a bulge for 400 nm $<x<$ 500 nm, to the right of the narrowest region. Only a small excess density appears in this bulge when $V_g=-0.724$ V [Figs. 2(b) and 2(c)], but a large density builds up at $V_g=-0.720$ V [Figs. 2(d) and 2(e)], revealing a resonant state. Electrons are forward scattered from one of the conducting modes into the extra mode that propagates within the bulge. They are reflected when this mode cuts off at the ends of the bulge to form the resonance. Some electrons are "forward" scattered out of the resonance into the backward-going conducting modes, giving an indirect backscattering process which lowers the conductance. Resonances can instead raise the conductance if electrons enter the resonance by tunneling rather than scattering.[7] These in-channel resonances should be distinguished from that seen in mode 3 of Fig. 1, which occurs when the mode is reflected at cutoff and does not affect the conducting states.

We have estimated some scattering lengths in this structure analytically using the Born approximation and

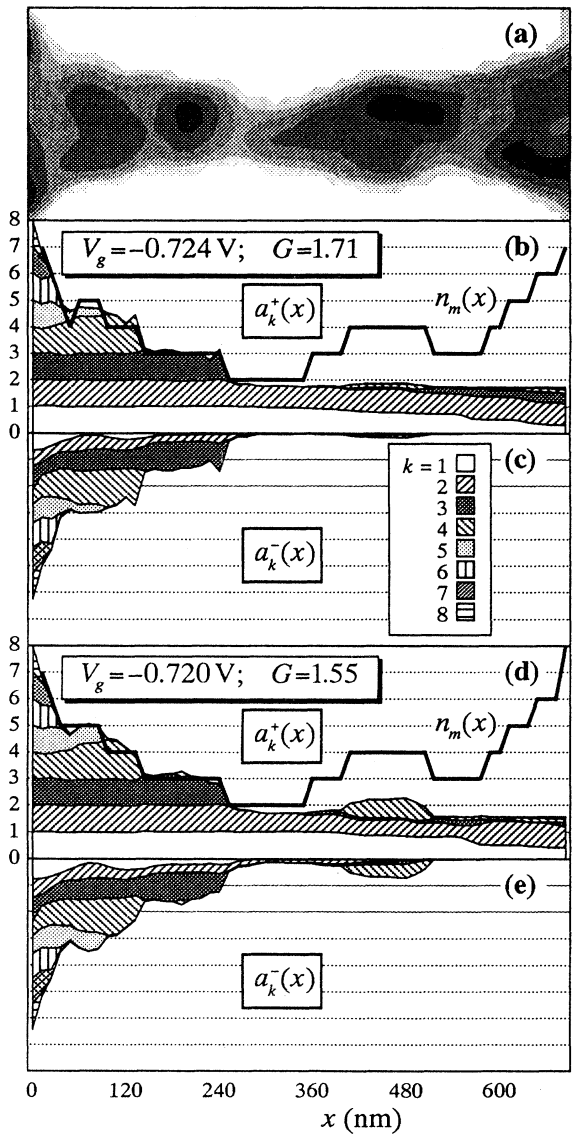

FIG. 2. Point contact with poorly quantized conductance. (a) Electron density with 4.2×10^{14} m^{-2} between levels of gray; (b) forward and (c) backward flux at $V_g=-0.724$ V, $G=1.71$, with $n_m(x)$ superposed on (b); (d) forward and (e) backward flux at $V_g=-0.720$ V, $G=1.55$, with $n_m(x)$ superposed on (d). Note the resonance within the bulge between 400 and 500 nm present in (d) and (e) but not in (b) and (c).

screened ionized impurity potentials. An unconfined 2DEG has a transport mean free path of 3.1 μm, while the unweighted mean free path is only 22 nm. There is a large difference because the random potential is slowly varying. For a wire confined in a parabolic potential with $\hbar\omega_0 + 1$ meV, which roughly models the point contact, the unweighted mean free path rises to 0.1 μm because scattering through very small angles is suppressed. Figure 1(f) shows that most electrons that enter the point contact in mode 1 travel less than 100 nm before being scattered out, in reasonable agreement. The transport mean free path, which includes only backscattering, rises to 10 μm.

None of these length scales tells us the maximum length of a point contact for good quantization, which experiment[9] and simulation[7] agree to be about $\frac{1}{4}$ μm. Moreover, the resonance in Fig. 2 makes it clear that the Born approximation cannot accurately describe scattering in this quasi-one-dimensional system. The problem is that successive scattering events are assumed to be independent, with no interference between them. It is known from field theory[12] that the assumption of independent scattering events fails in one dimension, and we believe that the resonant backscattering process provides a clear physical demonstration of this. We suggest that the maximum length of a point contact is set by the correlation length of the random potential— the size of a typical bulge—if resonances are indeed the dominant backscattering mechanism. This is about 0.2 μm for our potentials. This is in contrast to Glazman and Jonson,[13] who explain the breakdown of quantization entirely within the Born approximation. Our results also cast doubt on the prediction that electrons in narrow wires should have an enhanced mobility,[14] since this too was based on the Born approximation.

We have shown that the random potential in a real quantum point contact leads to rapid intermode scattering. The adiabatic approximation fails badly, but conductance can still be quantized subject to the less stringent requirement of "compensated" scattering. Resonances can cause strong backscattering and lead to poor quantization. They arise from the quasi-one-dimensional nature of the system, and show that scattering cannot be described within the Born approximation. The maximum length of a point contact for good quantization is set by the correlation length of the random potential if resonances provide the dominant backscattering.

We would like to thank J.M. Arnold, A.R. Long, H.U. Baranger, and J.W. Wilkins for useful discussions, and G. Timp for a copy of a stimulating article prior to publication. This work was supported by the United Kingdom Science and Engineering Research Council (M.J.L.) and Grants Nos. GR/E73192, GR/E18186, and GR/F80890. M.J.L. would also like to thank the Department of Electronics and Electrical Engineering at Glasgow University for additional financial support.

---

*Present address: Department of Physics, Paisley College of Technology, Paisley PA1 2BE, UK.

†Present address: Department of Physics, Ohio State University, Columbus, OH 43210-1106.

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

[2]D.A. Wharam, U. Ekenberg, M. Pepper, D.G. Hasko, H. Ahmed, J.E.F. Frost, D.A. Ritchie, D.C. Peacock, and G.A.C. Jones, Phys. Rev. B **39**, 6283 (1989).

[3]H. van Houten, C.W.J. Beenakker, and B.J. van Wees, in *Semiconductors and Semimetals,* edited by M.A. Reed (Academic, New York, (1991).

[4]P.A. Lee and D.S. Fisher, Phys. Rev. Lett. **47**, 882 (1981).

[5]L.I. Glazman, G.B. Lesovick, D.E. Khmel'nitskii and R.I. Shekhter, Pis'ma Zh. Eksp. Teor. Fiz, **48**, 218 (1988) [JETP Lett. **48**, 238 (1988)].

[6]J.A. Nixon and J.H. Davies, Phys. Rev. B **41**, 7929 (1990).

[7]J.A. Nixon, J.H. Davies, and H.U. Baranger, Phys. Rev. B (to be published).

[8]M.J. Laughton, J.M. Arnold, and J.R. Barker (unpublished).

[9]G. Timp, R. Behringer, S. Sampere, J.E. Cunningham, and R.E. Howard, in *Proceedings of the International Symposium on Nanostructure Physics and Fabrication, College Station, Texas,* edited by M. A. Reed and W. P. Kirk (Academic, New York, 1989), pp. 331–345.

[10]M.C. Payne, J. Phys. Condens. Matter **1**, 4939 (1989).

[11]M. Büttiker, Phys. Rev. B **41**, 7906 (1990).

[12]A.A. Abrikosov and I.A. Ryzhkin, Zh. Eksp. Teor. Fiz **71**, 1204 (1976) [Sov. Phys. JETP **44**, 630 (1976)].

[13]L.I. Glazman and M. Jonson (unpublished).

[14]H. Sakaki, Jpn. J. Appl. Phys. **19**, L735 (1980).