

Breakdown of quantized conductance in point contacts calculated using realistic potentials

John A. Nixon* and John H. Davies†

Department of Electronics and Electrical Engineering, University of Glasgow, Glasgow G12 8QQ, United Kingdom

Harold U. Baranger

AT&T Bell Laboratories, Murray Hill, New Jersey 07974

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Ionized donors in a heterostructure generate a random potential with long-ranged fluctuations. We have used realistic self-consistent potentials to study its effect on the quantized conductance of point contacts, and find that transport in confined and unconfined geometries probe complementary aspects of the random potential. Thus quantization breaks down when the length of the point contact exceeds $\frac{1}{2} \mu\text{m}$, an order of magnitude less than the mean free path in the bulk. The characteristics reflect the detailed configuration of impurities near the point contact.

The quantized conductance^{1,2} of narrow constrictions or “quantum point contacts” in a two-dimensional electron gas (2D EG) requires the low scattering rates achieved in heterostructures. A point contact behaves as a quasi-one-dimensional system and its conductance, in units of $(2e^2/\hbar)$, is given by the number of occupied transverse subbands.³ This can be controlled by the gate voltage. The transport mean free path in a heterostructure at low temperature, where it is limited by ionized impurity scattering, is typically many μm and the obvious inference is that the random potential must be very weak. It is therefore surprising to find⁴ that the quantization of conductance breaks down in point contacts longer than $\frac{1}{2} \mu\text{m}$ —an order of magnitude less than the mean free path. Must we invoke a different mechanism like electron-electron scattering, or is ionized impurity scattering still responsible? If so, it is clear that a point contact and an unpatterned 2D EG respond very differently to the random potential from the ionized impurities.

This raises the broader theoretical question: what aspects of the random potential are probed by different transport experiments? The natural first choice for a model is a sum of short-ranged potentials. This can be justified for three-dimensional metals, where screening is good and scattering is nearly isotropic. Different measures of disorder, such as the total and the transport scattering rates, are nearly identical, so the randomness can be characterized simply by a strength. However, the real random potential in a 2D EG from ionized donors is entirely different, because screening is poor and the donors are out of the plane. The impurity potentials are long ranged and overlap strongly in space, generating a random potential whose correlation length is long ($\approx 0.2 \mu\text{m}$) on the scale of the Fermi wavelength λ_F ($\approx 0.05 \mu\text{m}$), and much larger than the spacing between donors ($\approx 0.01 \mu\text{m}$).⁵ The ratio between λ_F and the correlation length explains the long mean free path of an unconfined 2D EG. However, other measures of disorder such as the width of Landau levels in a high magnetic field yield very

different scattering rates in such a potential.⁶

Here we show that the geometry of a transport experiment determines which features of the random potential are probed. In particular, the long-ranged nature of the potential is crucial in explaining the breakdown of the quantized conductance. This conclusion is based on calculations of the conductance of point contacts using realistic self-consistent potentials. We find that the conductance can be well quantized in short point contacts ($0.2 \mu\text{m}$), but scattering by the random potential destroys quantization in longer devices ($0.6 \mu\text{m}$) that exceed the correlation length. Even the $0.2 \mu\text{m}$ devices show evidence of the random potential, with large variations from device to device due to the specific configuration of donors near the active region. There are resonances in some samples, where the random potential produces a well under the point contact.

We have previously described a numerical technique to study the random potential caused by the ionized donors in patterned heterostructures,⁵ and have used the same semiclassical model to calculate the self-consistent potential for quantum point contacts. It includes the gates, which produce the guiding potential, and the randomly positioned ionized donors in the doped layer of the heterostructure, which provide the dominant scattering mechanism at low temperature. The main features of the model are as follows.⁷

(i) Donors are distributed at random in a δ -doped layer and are fully ionized. We ignore other impurities, parallel conduction, DX centers, and possible correlation between the positions of donors.

(ii) Electrons are treated as a strictly two-dimensional gas whose density is given by a local, semiclassical Thomas-Fermi approximation.

(iii) The chemical potential is perfectly pinned on the surface.

The conductance of electrons through the self-consistent potential is then found quantum mechanically. Perfect leads, in which no scattering occurs, are attached to the system by extending the potential profile at the left

and right edges outward to infinity. The Green's function for an electron is then calculated recursively.⁸ This method is applicable to any random potential, and is equivalent to solving the Schrödinger equation using finite differences. The conductance G was found from the transmission matrix t using $G = (2e^2/h) \text{Tr}(tt^\dagger)$. The calculation was performed for zero temperature.

We modeled the devices of Timp *et al.*,⁴ which had the following layers: metallic patterned gate; undoped cap of GaAs, 6 nm thick; undoped $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$, 24 nm thick; δ -doped layer with $N_D^{(2D)} = 4 \times 10^{16} \text{ m}^{-2}$; undoped spacer of $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$, 42 nm thick; undoped substrate of GaAs.

Si in $\text{Al}_{1-x}\text{Ga}_x\text{As}$ does not behave as an ideal donor and only a fraction ionizes, so the full value of doping $N_D^{(2D)}$ would give an excessively large electron density. The doping was therefore reduced to $2.5 \times 10^{16} \text{ m}^{-2}$ in the simulation. This gave around $3 \times 10^{15} \text{ m}^{-2}$ electrons when the gate is unbiased, comparable with the experimental value of $2.75 \times 10^{15} \text{ m}^{-2}$. We simulated both patterns of point contacts: each has a gap $g = 0.3 \mu\text{m}$ between the gates, with lengths $l = 0.2$ and $0.6 \mu\text{m}$. The calculations were performed with several configurations of the discrete, random impurities. For comparison, we also considered smooth potentials obtained by replacing the

discrete impurities with a sheet of uniform charge density.

Contour maps of typical electron densities are shown in Fig. 1. These can also be viewed as potential-energy plots showing only the contours below the Fermi energy. Figure 1(a) shows the $0.2\text{-}\mu\text{m}$ -long gate with a smooth potential. The point contact has an ideal saddle point, and transport should be described well by the adiabatic approximation.⁹ Figure 1(b) shows a realistic case including the random potential. The saddle point is shifted by the impurities but is not greatly distorted. In contrast, Fig. 1(c) shows the $0.6\text{-}\mu\text{m}$ point contact, which is longer than the correlation length of the random potential. There are now fluctuations within the point contact, which are likely to cause scattering. The potential gets rougher as the channel is squeezed further and the density of electrons is reduced, as seen before in wires.⁵

The calculated conductances G as a function of gate voltage V_g are plotted in Fig. 2. In Fig. 2(a), for the $0.2\text{-}\mu\text{m}$ gate, curve A shows the good quantization of the smooth system. The rounded guiding potential [Fig. 1(a)]

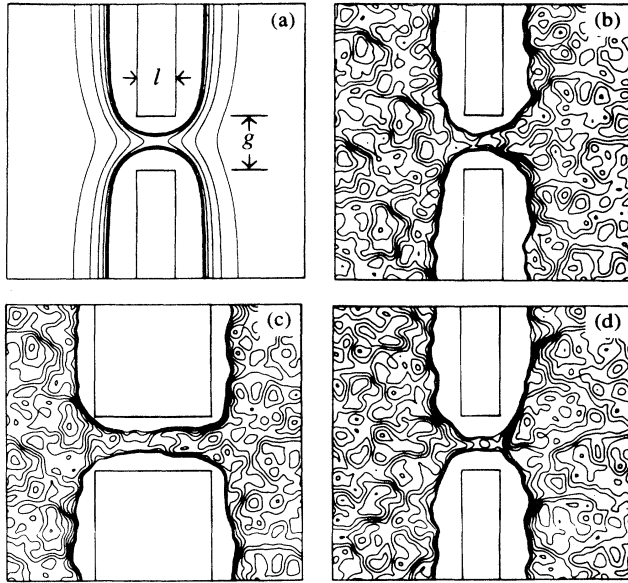


FIG. 1. Gate pattern on surface and density of electrons in 2D EG for point contacts with $g = 0.3 \mu\text{m}$, and $l = 0.2$ and $0.6 \mu\text{m}$. Contours start from zero and are $4.2 \times 10^{14} \text{ m}^{-2}$ apart, corresponding to an energy spacing of 1.5 meV . All cases correspond to two transverse subbands being occupied in the neck of the point contact. The effect of the random potential for the $0.2\text{-}\mu\text{m}$ gate is seen by comparing (a), in which there are no random donors and the contours are smooth, with (b) in which the impurity potential is present. The $0.6\text{-}\mu\text{m}$ gate in (c) exceeds the correlation length of the random potential, and there are fluctuations within the point contact. (d) Shows a potential well in the channel which contains a resonance.

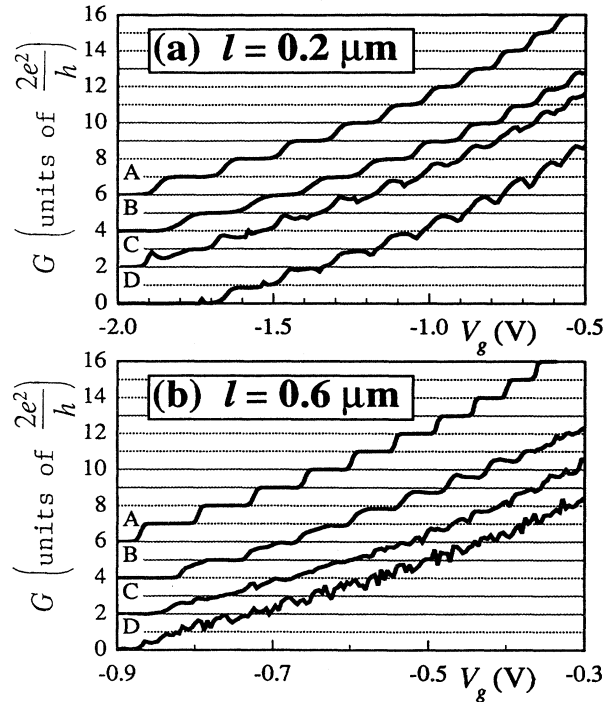


FIG. 2. Conductance G as a function of gate voltage V_g for (a) the $0.2\text{-}\mu\text{m}$ gate and (b) the $0.6\text{-}\mu\text{m}$ gate. Curves are offset for clarity. Curve A in each case shows the clean quantized steps found in a smooth system. The other curves are for different impurity configurations, showing a variety of characteristics. For the $0.2\text{-}\mu\text{m}$ gate the conductance can be well quantized, with six good steps shown in curve B. Curves C and D show structure due to resonances in the channel. The breakdown in quantization in a longer point contact is shown by curves B–D in (b), with one plateau at best. Curve A in (a) is for the sample illustrated in Fig. 1(a); B in (a) corresponds to Fig. 1(b); B in (b) to Fig. 1(c); and D in (a) to Fig. 1(d).

prevents “organ-pipe” resonances¹⁰ from developing. Curve *B* shows that G can remain well quantized even in the presence of the random potential, although the steps between plateaus are broadened. Another sample, not shown here, also shows good quantization. Curves *C* and *D*, for two other configurations, are poorly quantized with structure due to the random potential which will be discussed below. For the $0.6\text{-}\mu\text{m}$ point contact in Fig. 2(b) the smooth potential shows better quantization than the shorter point contact because tunneling through the saddle point is reduced (curve *A*). Including the random potential reverses this, and quantization is much poorer than in the shorter point contact (curves *B–D*). No sample shows more than one good plateau because of back-scattering by the random potential in the point contact. In most cases there is almost no remnant of the steps, in agreement with experiment.⁴

We have seen resonances within the channel of the shorter device. Curve *D* in Fig. 2(a) shows sharp peaks in $G(V_g)$ below the onset of the first and second plateaus. The density of electrons is plotted in Fig. 1(d) for $V_g = -1.53\text{ V}$, and shows a clear double barrier in the point contact.¹¹ This is produced by a well in the *random* potential, in contrast to devices where a patterned gate has been used deliberately to produce a “quantum dot.”¹² The resonance broadens and disrupts the higher plateaus: resonant *tunneling* turns into resonant *backscattering*, which has been explained using a coupled-mode analysis by Laughton *et al.*¹³ Somewhat similar resonances have been seen in calculations with short-ranged attractive potentials.^{14,15} Features in the potential can be explored experimentally by scanning the point contact with a differential bias.¹⁶

Several effects are introduced if the temperature is raised above zero: (i) the density of electrons changes; (ii) the distribution function broadens; and (iii) inelastic scattering starts. We do not expect (i) to be important as we are only interested in temperatures below 4.2 K , and (iii) is very difficult to treat realistically. We have estimated the effect of (ii), a broadened distribution function, to see if this alone can explain the experimental observation that the quantized steps disappear above 1 K . The conductance as a function of energy $G(E)$ must be averaged over the derivative of the Fermi function $(-\partial f/\partial E)$. We used $G(E_F)$ as an estimate of $G(E)$, where E_F is the Fermi energy of electrons at the narrowest point of the point contact and depends on V_g . The results for one of the $0.2\text{-}\mu\text{m}$ samples [curve *D* of Fig. 2(a)] are shown in Fig. 3. A small increase in temperature (0.5 K) smooths the fine detail of the resonant structure. More detail is lost as the temperature increases, but the plateaus become better defined; experimentally they are best near 0.5 K .¹ The plateaus themselves disappear due to thermal smearing when the subband spacing becomes comparable to $4k_B T$, and there is no trace of them at 4.2 K in this device. Although there must be some inelastic scattering at this temperature, it need not play a major role in the disappearance of the quantized conductance: thermal broadening alone seems

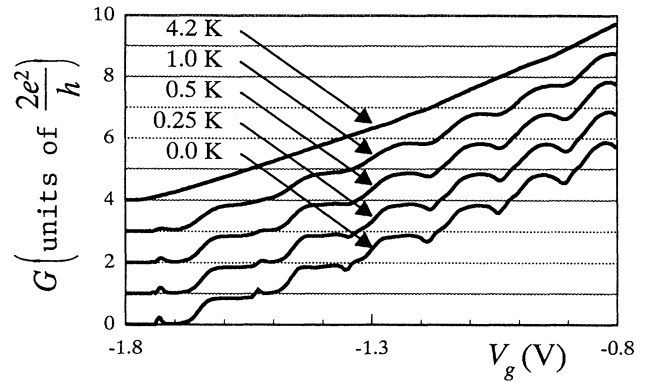


FIG. 3. $G(V_g)$ for a $0.2\text{-}\mu\text{m}$ device [curve *D*, Fig. 2(a)] and a range of temperatures. Details of the resonance are lost by thermal smearing as the temperature is raised to 0.5 K , but the quality of the plateaus improves. The quantized steps lose definition at higher temperatures and vanish by 4.2 K .

to be sufficient.

A general comparison of our results with experimental data suggests that we overestimate the size of the fluctuations by a small factor. Our treatment of the donors is almost certainly responsible. The first problem is the assumption that all donors are ionized. We pointed out earlier that this leads to a much higher density of electrons than that seen experimentally. Also, thermal cycling of devices to room temperature produces different conductance characteristics when the measurements are repeated at low temperature,¹⁷ which is thought to be due to a redistribution of ionized donors. Secondly, there may be correlation between the positions of *ionized* donors, although the donors as a whole are placed at random.¹⁸ We intend to include these effects and the “back-ground” impurities in our model.

We have shown that the mobility of a uniform 2D EG and the quality of quantization in a point contact reflect complementary aspects of the random potential. The long range of fluctuations in a doped heterostructure explains why quantization breaks down in point contacts longer than $\frac{1}{2}\mu\text{m}$, while the “bulk” mean free path is many μm . The active region of $0.2\text{ }\mu\text{m}$ point contacts is comparable with the correlation length of the random potential, leading to large variations between nominally identical devices even if they are fabricated perfectly. These variable characteristics set a fundamental physical limitation on the performance of ultrasmall devices based on doped heterostructures.

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- *Present address: Department of Physics, Paisley College of Technology, Paisley PA1 2BE, United Kingdom.
- †Present address: Department of Physics, Ohio State University, Columbus, OH 43210-1106.
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