On the possibility of direct observation of the difference between cyclic and zero boundary conditions

1990 J. Phys.: Condens. Matter 2 5271

(http://iopscience.iop.org/0953-8984/2/23/019)

J. Phys.: Condens. Matter 2 (1990) 5271–5275. Printed in the UK

LETTER TO THE EDITOR

On the possibility of direct observation of the difference between cyclic and zero boundary conditions

A M Zagoskin and I O Kulik
Institute for Low Temperature Physics and Engineering, 47 Lenin Avenue, Kharkov 310164, USSR

Received 4 April 1990

Abstract. The two-dimensional point contacts formed in the inversion layer of GaAs–AlGaAs heterojunctions demonstrate steps in their conductance versus gate potential dependence. It is shown that the step structure depends on the topology of the contact which can be changed from one corresponding to zero boundary conditions, to that appropriate for cyclic ones. The step structure would follow the relation $G = (2e^2/h)n$ in the first and $G = (2e^2/h)(2n + 1)$ in the second case ($n = 0, 1, 2, \ldots$).

It is well known that the cyclic boundary conditions conventionally used in solid state physics to eliminate the surface influence result in simple characterisation of the energy levels for finite periodic systems. The applicability of these conditions to macroscopic systems is justified by the fact that they give correct values of bulk observables, e.g., the number of states per site. Nevertheless, these two types of boundary condition describe systems with different topologies. To demonstrate the qualitative difference between them we need a system in which we can change the boundary condition from cyclic to zero and vice versa and compare results. We shall show that the two-dimensional point contact of a special geometry can be such a system: quantisation of its conductance qualitatively depends on its topology.

It was shown in recent papers [1, 2] that the conductance of a two-dimensional electron gas (2DEG) flowing through a junction of diameter d, as a function of d, displays steps of magnitude $2e^2/h = (12.912\ \mathrm{k\Omega})^{-1}$. A simple explanation of the effect is based upon quantisation of the transverse momentum of an electron in the contact region.

The conductance is given by the formula

$$G(d) = \frac{2e^2}{h} \sum_n T_n(d) \tag{1}$$

in which $T_n(d)$ ($0 \leqslant T_n \leqslant 1$) is the filling number of the nth transverse mode existing in the contact. This quantity can also be regarded as the transparency of the nth conducting channel, so that (1) is interpreted as the multichannel version of Landauer's formula [3],

0953-8984/90/235271 + 05 $03.50

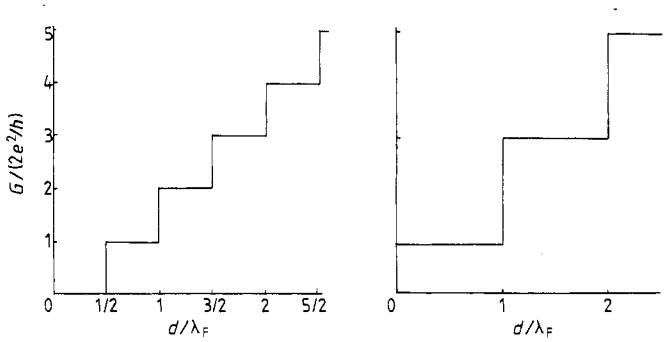

Figure 1. Conductance quantisation in an infinitely long channel of width d: (a) zero boundary condition, (b) cyclic boundary condition.

without interchannel scattering (see [4]). If the contact is modelled by an infinitely long channel of width d, then the wave function of the nth transverse mode is

$$\phi_n(x) = (2/d)^{1/2} \sin(\pi n x/d). \tag{2}$$

It corresponds to the energy

$$E_n(d) = (hn/2d)^2/2m \qquad (n = 1, 2, \ldots). \tag{2a}$$

If, on the contrary, we choose the cyclic boundary conditions then

$$\phi_n^{\pm}(x) = (d)^{-1/2} \exp(\pm 2\pi i n x/d) \tag{3}$$

and the energy equals

$$E_n^{\pm}(d) = (hn/d)^2/2m \qquad (n = 0, 1, 2, \ldots). \tag{3a}$$

Let us suppose that the connection of our channel to the electronic reservoirs is adiabatic. Then, the value of T_n is

$$T_n(d) = \theta(\varepsilon_F - E_n(d))$$

where $\theta(x)$ is the Heavyside step function, and (1) can be rewritten in the form

$$G(d) = (2e^2/h) \sum_E \nu_E \theta(\varepsilon_F - E(d)). \tag{4}$$

ν_E is the multiplicity of the energy level E. The dependence G upon d has steps in both cases but the character of the step differs.

The case of the zero boundary condition has been discussed in [1, 2]. It is clear from (4) that G has steps of the magnitude $2e^2/h$ each time d is increased by $\lambda_F/2$ (see figure 1(a)), and the first step develops at $d = \lambda_F/2$.

In the case of cyclic boundary conditions the picture is different. Since the transverse energy levels are twice degenerate, $G(d)$ has $4e^2/h$ steps when d is increased by λ_F (figure 1(b)). The only non-degenerate level ($n = 0$) produces a $2e^2/h$ step beginning at $d = 0$. This does not mean that the channel of zero width has finite conductance because such a channel cannot be adiabatically connected with the reservoirs. Therefore the first step will be smoothed out but the behaviour of the conductance at $d \to 0$ in the case of the cyclic boundary conditions is clearly different from that for zero ones.

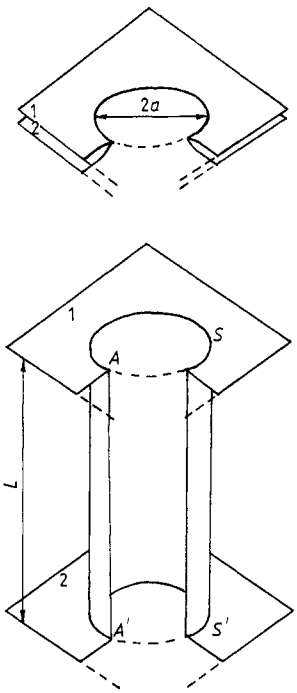

Figure 2. Exactly solvable configuration for a two-dimensional point contact. (*a*) Glueing of two planes in an attempt to allow for conductance from one to another. (*b*) Cylindrical surface connecting two planes.

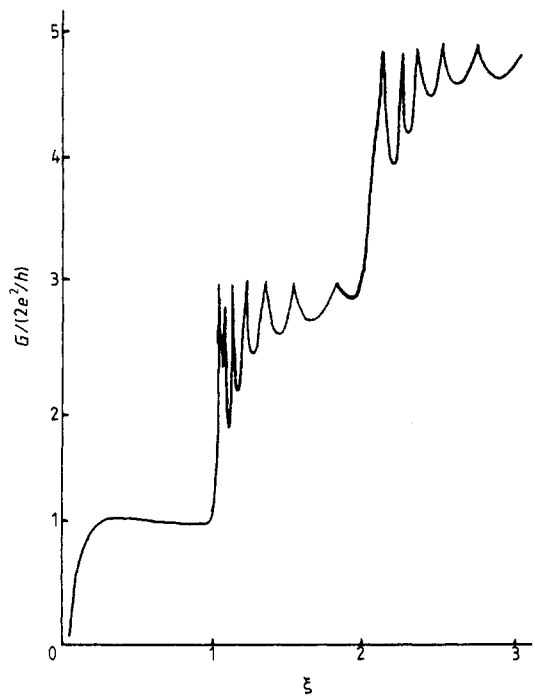

Figure 3. Conductance versus dimensionless contact radius $\xi = k_F a$ (at $\eta \equiv k_F L = 40$).

Let us clarify the above speculation by considering an exactly solvable model of a two-dimensional ballistic point defect [5]. As was shown by approximate solution [6] of the Schrödinger equation for the contact shaped as a rectangular channel, the conductance has $2e^2/h$ steps with resonant structure due to electron reflection at sharp edges of the channel. If we roll the rectangular channel into a tube, and glue its edges to planes having orifices of the same diameter, the configuration shown at figure 2, we shall obtain geometry of a contact subject to the cyclic boundary conditions with respect to the transverse coordinate, $x = R\theta$ (θ is the azimuthal angle).

Since the system is radially symmetric, the Schrödinger equation can be solved exactly. The boundary conditions at circles S and S' connecting the planes with the tube are

$$\begin{cases} \Psi_k^{(1)}(r,\theta) = \Psi_k^{(C)}(z,\theta)\Big|_{\substack{r=a\\z=L}} \equiv \Psi_L(\theta) \\ \dfrac{\partial}{\partial r}\Psi_k^{(1)}(r,\theta) - \dfrac{\partial}{\partial z}\Psi_k^{(C)}(z,\theta)\Big|_{\substack{r=a\\z=L}} = \dfrac{8\pi^2 m^* U}{h}\Psi_L(\theta) \\ \Psi_k^{(2)}(r,\theta) = \Psi_k^{(C)}(z,\theta)\Big|_{\substack{r=a\\z=0}} \equiv \Psi_0(\theta) \\ \dfrac{\partial}{\partial r}\Psi_k^{(2)}(r,\theta) + \dfrac{\partial}{\partial z}\Psi_k^{(C)}(z,\theta)\Big|_{\substack{r=a\\z=0}} = \dfrac{8\pi^2 m^* U}{h}\Psi_0(\theta). \end{cases} \tag{5}$$

The second and fourth lines provide for preservation of the current; $U > 0$ can be regarded as the magnitude of the effective δ-potentials uniformly distributed along S, S'. The wave function of an electron propagating from the upper plane to the orifice is

$$\Psi_k^{(1,2)} = \sum_{n=-\infty}^{\infty} \mathrm{i}^n \chi_n(kr)\, \mathrm{e}^{\mathrm{i}n\theta} \tag{6}$$

where

$$\begin{cases} \chi_r^{(1)}(kr) = J_n(kr) + \dfrac{\rho_n - 1}{2}\,(J_n(kr) + \mathrm{i}N_n(kr)) \\ \chi_r^{(2)}(kr) = \frac{1}{2}\tau_n(J_n(kr) + \mathrm{i}N_n(kr)). \end{cases} \tag{7}$$

J_n, N_n are the Bessel and Neumann functions, respectively.

The wave function $\Psi_k(r, \theta)$ consists of a plane wave with the wavevector $\boldsymbol{k}$, supplemented by a scattered wave in the upper bank, and a diverging wave in the lower bank.

The wave function on the cylindrical surface is

$$\Psi_k^{(C)}(z, \theta) = \sum_n [c_n^+ \exp(\omega_n(\xi)\eta) + c_n^- \exp(-\omega_n(\xi)\eta)\, \mathrm{e}^{\mathrm{i}n\theta} \tag{8}$$

where $\xi = k_F a$ and $\eta = k_F L$ are the dimensionless radius and the length of the contact, respectively, and $\omega_n(\xi) = \mathrm{i}[1 - (n/\xi)^2]^{1/2}$. The coefficients ρ_n, τ_n and $c_n^{\pm}$ are determined by the solution of (5).

The conductance of the contact in the limit $V \to 0$ (where eV is the contact bias) is represented as

$$G = (2e^2/h)\left(T_0 + 2\sum_{n=1}^{\infty} T_n\right) \tag{9}$$

where $T_n = |\tau_{\pm n}(\xi)|^2$, $0 < T_n < 1$. The solution for T_n reads

$$T_n(\xi, \eta) = [(8/\pi\xi)^2 |\omega_n(\xi)|^2 / |\cosh(\omega_n(\xi)\eta)|^2] \left| 2\tanh(\omega_n(\xi)\eta)\left[\left(\frac{\mathrm{d}}{\mathrm{d}\xi} H_n^{(1)}(\xi)\right)^2 \right.\right.$$

$$\left.\left. + \omega_n^2(\xi)(H_n^{(1)}(\xi))^2\right] - 2\omega_n(\xi)\frac{\mathrm{d}}{\mathrm{d}\xi}(H_n^{(1)}(\xi))^2 \right|^{-2} \tag{10}$$

where $H_n^{(1)}(\xi)$ is the Hankel function. For simplicity we put $U = 0$.

It can easily be shown that for a sufficiently long cylinder the conductance as a function of ξ has steps with resonant structure, the total number of which (before the steps smoothen out) is of the order of $N \simeq 13\,(L/\lambda_F)^2$ (at $T = 0$). As is seen from figure 3, the first step is quite sharp at small a. The resonant structure of the step is similar to that discussed in [6]. If we 'cut' the cylinder along the line AA, the picture will change into the 'zero' pattern with $2e^2/h$ steps (figure 1).

These considerations allow us to suggest a direct experimental demonstration of the difference between the cyclic and zero boundary conditions. The configuration of figure 3 can be realised, for example, as an inversion layer on two sides of an isolated flat metal

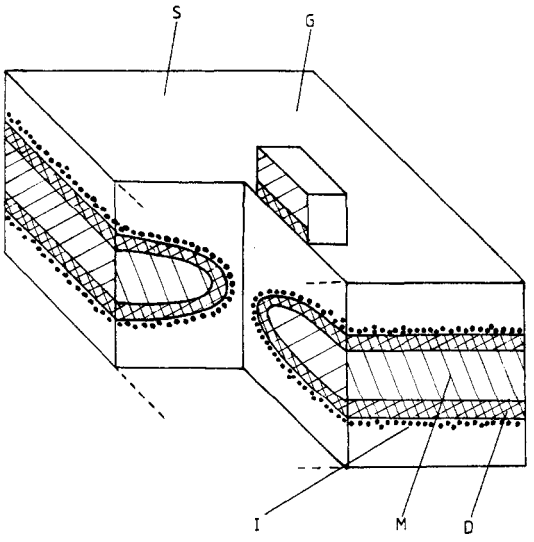

Figure 4. Scheme of the proposed experimental demonstration of the difference between the zero and cyclic boundary conditions. M is the metal mask, S a semiconductor, D the insulating layer. I is the inversion layer, and G the metallic electrode (a gate).

mask M with an orifice of the radius a, imbedded into a semiconductor S (figure 4). The effective radius of the contact $\xi = k_F a$ depends on the potential applied to M. The negative potential on the gate G will 'cut' the cylindrical layer and qualitatively change the form of the dependence $G(\xi)$ from being $2e^2/h$ step-like to $4e^2/h$ step-like.

We are grateful to Dr R I Shekhter and Dr E N Bogachek for helpful discussions.

References

[1] van Wees B J, van Houten H, Beenakker C W J *et al* 1988 Quantized conductance of point contacts in a two dimensional electron gas *Phys. Rev. Lett.* **60** 848–50
[2] Wharam D A, Thornton T J, Newbury R *et al* 1988 One-dimensional transport and the quantisation of the ballistic resistance *J. Phys. C: Solid State Phys.* **21** L209–14
[3] Landauer R 1970 Electrical resistance of disordered one-dimensional lattices *Phil. Mag.* **21** 863–7
[4] Imry Y 1986 Physics of mesoscopic systems *Directions in Condensed Matter Physics* ed G Grinstein and G Mazenko (Singapore: World Scientific) pp 101–63
[5] Zagoskin A M and Kulik I O 1990 Quantum oscillation of the electrical conductance of two-dimensional ballistic contacts *Fiz. Nizk. Temp.* **16** at press
[6] Szafer A and Stone A D 1989 Theory of quantum conduction through a constriction *Phys. Rev. Lett.* **62** 300–3