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LETTER TO THE EDITOR

Geometric criterion for accurate conductance quantization in a lateral constriction

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Abstract. A novel approach to conductance quantization is presented, based on the reduction of the problem of electron motion in a ballistic constriction of arbitrary shape to a problem with separable variables. The approach gives a simple geometric criterion for accurate quantization in the plateau regions as well as sharp changes in conductance from one plateau to the next with varying minimal constriction width. The criterion is that at any point along the boundary, the constriction width must be much smaller than the radius of curvature of the boundaries. In a system satisfying the criterion, an electron wave propagates through the entire device without mode mixing, and new channels of propagation switch on and off sharply.

The problem of ballistic transport in small devices of different geometries has recently received considerable attention [1] following the discovery of conductance quantization in lateral constrictions [2–4]. Most theoretical papers have so far used numerical methods [5–6]. Results obtained by these methods depend strongly on the exact shape of the boundaries, and do not point to any clear criterion for accurate quantization in a constriction of arbitrary shape. The only systematic approach to conductance quantization reported so far, giving (at least in principle) corrections of any desired accuracy, is the adiabatic approximation [7, 8]. This approximation is plagued, however, by the well known difficulties in the explicit extraction of a small expansion parameter. Another essential shortcoming is the breakdown of this approximation (and of models used in [5]) in regions where the constriction connects to reservoirs (as discussed by Landauer [9]), where the width, generally speaking, is unlimited.

In the present paper, a novel approach to conductance quantization is presented which is free of the above limitations. It is based on the reduction of the problem of electron motion in a constriction of arbitrary shape to a problem with separable variables. The new coordinates are defined by curvilinear trajectories along and across the constriction. These correspond to equipotential lines and lines of force in a curvilinear condenser and are uniquely determined by the shape of the constriction. Separation is possible if at every point the width d of the constriction, defined as the length of the trajectory across the constriction (figure 1(a)), is much less than the radius of curvature of the boundaries r. When this condition is met, an electron wave propagates through the entire device without mode mixing, allowing accurate conductance quantization in the plateau regions. Furthermore, the condition guarantees abrupt switching on of new propagation channels when the minimal constriction width

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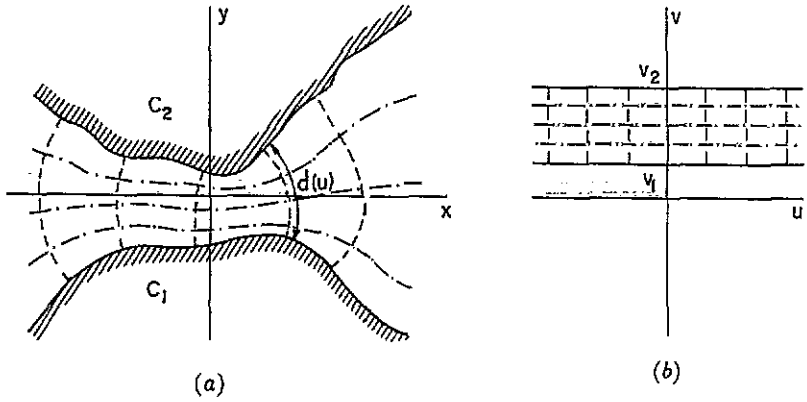

Figure 1. Definition of the width for a constriction of arbitrary shape (*a*) by means of conformal mapping into a straight band (*b*). u- and v-coordinate lines are shown by dashed and dot-dashed curves respectively.

is increased, leading to a sharp change from one plateau to the next. The condition $d/r \ll 1$ is easily satisfied even far from the narrowest part of the constriction, where the adiabatic approximation breaks down. Moreover, for a smooth enough constriction, where a semiclassical approximation may be used, the strong cancellations in the integrals due to the varying phases of the WKB exponentials introduce exponentially small coefficients into the higher-order corrections in d/r.

Consider a lateral constriction of arbitrary shape (figure 1(*a*)) with a square-well confining potential. Electron motion inside the well is free and obeys the Schrödinger equation $\Delta\Psi(x,y) + k^2\Psi(x,y) = 0$, where $\Psi(x,y)$ is the electron wavefunction, $\Delta = \partial^2/\partial x^2 + \partial^2/\partial y^2$, $k^2 = 2mE$ is the wavenumber and $\hbar = 1$. Interaction with the walls yields the boundary conditions $\Psi(C_1) = \Psi(C_2) = 0$.

Any simply connected domain (e.g. figure 1(*a*)) can be conformally mapped into a straight band (figure 1(*b*)) [10]. The appropriate analytical function, $\omega = f(z)$ ($\omega = u + \mathrm{i}v$; $z = x + \mathrm{i}y$) transforms boundaries, C_1 and C_2 to the straight lines $v = v_1$ and $v = v_2$, respectively. In the orthogonal curvilinear coordinates (u,v) the Schrödinger equation and the boundary conditions take the form [11]

$$\Delta\Psi(u,v) + k^2 e^2(u,v)\Psi(u,v) = 0 \qquad \Psi(u, v_0 \pm \Delta v/2) = 0 \quad (1)$$

Here $\Delta = \partial^2/\partial u^2 + \partial^2/\partial v^2$, $e(u,v) = |\mathrm{d}z/\mathrm{d}\omega|$ is the variable scale factor determining the length $\mathrm{d}s^2 = e^2(u,v)(\mathrm{d}u^2 + \mathrm{d}v^2)$, $v_0 = (v_2 + v_1)/2$ and $\Delta v = v_2 - v_1$. Equation (1) describes the motion of an electron with variable effective mass, $m(u,v) = me^2(u,v)$, in the strip (figure 1(*b*)).

The above transformation is widely used in solving Laplace equations in electrostatics. There the v-coordinate lines lie along equipotential lines, and the u-coordinate lines lie along lines of force.

We now define the constriction width as the length of the u-coordinate line section between the walls: $d(u) = \int_{v_1}^{v_2} \mathrm{d}v\, e(u,v)$ (figure 1(*a*)). Defined in this fashion, the width pattern is uniquely set by the shape of the constriction and does not depend on the choice of the reference coordinate system (x,y). The radius of curvature, $r_v(u)$, of the v-coordinate line is given by $\frac{1}{r_v(u)} = \frac{\mathrm{d}}{\mathrm{d}v}\frac{1}{e(u,v)}$ [12].

The width and the curvature, as defined above, uniquely determine the effective mass and thus the dynamics of an electron. Variables $d(u)$, $r_v(u)$ and $e(u,v)$ are

connected by the relation

$$\int_{v_1}^{v_2} \frac{\mathrm{d}v'}{\int_v^{v'} \frac{\mathrm{d}v''}{r_{v''}(u)} + \frac{1}{e(u,v)}} = d(u)$$

yielding

$$e(u,v) = \frac{d(u)}{\Delta v}\left(1 + \frac{d(u)}{r(u,v)}\right)$$

when

$$\gamma(u) = \max_{v_1 \leqslant v, v' \leqslant v_2} \frac{d(u)}{\Delta v}\left|\int_v^{v'} \frac{\mathrm{d}v''}{r_{v''}(u)}\right| \ll 1.$$

Here

$$\frac{1}{r(u,v)} = \int_{v_1}^{v_2} \frac{\mathrm{d}v'}{\Delta v} \int_v^{v'} \frac{\mathrm{d}v''}{\Delta v} \frac{1}{r_{v''}(u)}.$$

Denoting the minimal radius of curvature

$$r(u) = \min_{v_1 \leqslant v \leqslant v_2} |r_v(u)|$$

one obtains $|r(u,v)| \geqslant 2r(u)$ and $\gamma(u) \leqslant d(u)/r(u)$. $r(u)$ corresponds, in many practical cases, to one of the boundaries.

Thus, to leading order in the small parameter $\gamma(u) \ll 1$, the effective mass $m(u,v)$ does not depend on v and the variables in equation (1) are separated. Such separation corresponds to the separation of motion along u- and v-coordinate lines in real space (figure 1(*a*)).

Let us demonstrate how the inequality $\gamma(u) \ll 1$ is satisfied in two examples; symmetric hyperbola boundaries [6, 13] and co-focal parabola boundaries. In the first case, $e(u,v) = c(\cosh^2 u - \cos^2 v)^{1/2}$, $v_1 = \alpha$, $v_2 = \pi - \alpha$ and the equation of v-coordinate lines is

$$\frac{y^2}{c^2 \cos^2 v} - \frac{x^2}{c^2 \sin^2 v} = 1.$$

This yields

$$\gamma(u) \leqslant \left(1 - \frac{\cos^2 \alpha}{\cosh^2 u}\right)^{-1/2} - 1$$

i.e. $\gamma(u) \ll 1$ for any u when $\cos^2 \alpha \ll 1$ and for any α when $\cosh^2 u \gg 1$. In the second case, $e(u,v) = (u^2 + v^2)^{1/2}$, $v_1 = \sqrt{a}$, $v_2 = \sqrt{b}$ and the equation of v-coordinate lines is

$$y = \frac{x^2}{2v^2} - \frac{v^2}{2}.$$

This yields

$$\gamma(u) \leqslant \left(\frac{u^2+b}{u^2+a}\right)^{1/2} - 1$$

i.e. $\gamma(u) \ll 1$ for any u when $(b-a) \ll a$ and for any a and b when $u^2 \gg b$. Thus the separation of the variables is surprisingly easy to justify far from the narrowest part of the constriction and the contact resistance is much less of a problem than was expected (cf [13]).

To describe electron motion along the constriction it is convenient to change variables from u to $s_v = \int_{u'}^{u} \mathrm{d}u\, e(u,v)$, which is the length of the v-coordinate line section between points u and u'. The 'average' distance along the constriction is

$$s = \frac{1}{\Delta v}\int_{v_1}^{v_2} \mathrm{d}v\, s_v = \frac{1}{\Delta v}\int_{u'}^{u} \mathrm{d}u\, d(u).$$

Introducing the function $\Phi(s,v) = (d(u)/\Delta v)^{1/2}\Psi(u,v)$, the solution of equation (1) can be written in the form $\Phi(s,v) = \sum_{n=1}^{\infty} C_n(s)F_n(v)$, which satisfies the boundary conditions. Here $F_n(v) = \sqrt{2/\Delta v}\sin\left(n\pi\left(\frac{v-v_0}{\Delta v}+\frac{1}{2}\right)\right)$. Substituting into (1) yields

$$C_n'' + k_n^2 C_n + \sum_m W_{nm} C_m = 0. \tag{2}$$

Here the primes denote the derivative with respect to s, $n = 1,2\ldots$ is the mode (channel) number,

$$k_n^2 \equiv k_n^2(s) = k^2 - \left(\frac{n\pi}{d(s)}\right)^2 + \frac{(d_s')^2 - 2d(s)d_s''}{4d^2(s)}$$

is the longitudinal wavenumber and

$$W_{nm} \equiv W_{nm}(s) = \int_{v_1}^{v_2} \mathrm{d}v\, F_n(v)W(s,v)F_m(v)$$

where $W(s,v) = k^2 2d(s)/r(s,v)$ describes the mode coupling. Now one can solve equation (2) by iterations with respect to the small parameter $d(s)/r(s) \ll 1$.

In the leading approximation, equation (2) describes the motion of an electron along u- and v-coordinate lines without mode mixing. If $d(s)$ varies slowly enough, then one can use the semiclassical solution of equation (2),

$$C_n^{\pm}(s) \sim (k_n(s))^{-\frac{1}{2}} \exp\left(\pm \mathrm{i}\int^{s} \mathrm{d}s\, k_n(s)\right)$$

relating to the left-coming (+) and to the right-coming (−) waves. Thus for the nth channel the problem is reduced to the WKB treatment of electron motion in the effective potential $V_n(s) = \frac{1}{2m}(n\pi/d(s))^2$. Reflection R and transmission T coefficients are diagonal with respect to the channel number and can be obtained by standard methods [14].

The bottleneck acts as a potential barrier. For channels with $n < n_{\min} = (kd_{\min}/\pi)$ ((x) is the integral part of x; $d_{\min} = d(s_0)$ is the minimal width of the constriction), an electron undergoes above-barrier reflection. If only two conjugated turning points $k_n(s \pm is') = 0$ exist, then one can use the Kembel formula,

$$T_n = 1 - R_n = \left[1 + \exp\left(-2\int_{s-is'}^{s+is'} dx' \, |k_n(s + ix')|\right)\right]^{-1}$$

yielding the exact result for a parabolic potential. If $n = n_{\min}$ in the vicinity of the barrier top, where the effective potential may be approximated by a parabolic one, then the Kembel formula yields

$$T_n = \left[1 + \exp\left(-\frac{k_n^2 d_{\min}}{n}\sqrt{\frac{d_{\min}}{d''_{s_0}}}\right)\right]^{-1}. \tag{3}$$

If $n > n_{\min}$ for sub-barrier transmission, then

$$T_n \sim \exp\left(-2\int_{s_1}^{s_2} ds \, k_n(s)\right)$$

where $k_n(s_{1,2}) = 0$. Since channels with $n \leqslant n_{\min}$ have $T_n \approx 1$ and the others have $T_n \ll 1$, it follows that only $n_{\min}$ channels give significant contributions to the conductivity $G = (e^2/\pi)\sum_n T_n$. Step-like changes in $n_{\min}$ as a function of $kd_{\min}$ cause the conductance quantization [2, 3]. The shape of the steps in G is determined by (3), giving

$$\delta G(z) = (e^2/\pi)\left[1 + \left(\exp(-2\pi^2 z/\sqrt{d_{\min} d''_{s_0}}\right)\right]^{-1}$$

where $z = (kd_{\min}/\pi) - n_{\min} \leqslant 1$ (cf [7]). Because $d''_{s_0} \leqslant 2/r(s_0)$, the condition $d(s) \ll r(s)$ provides not only accurate quantization in the plateau region, where $G = (e^2/\pi)n_{\min}\left[1 + n_{\min}O((d/r)^2)\right]$, but also guarantees very small widths of steps between adjacent plateaus ($|z| < \frac{1}{2\pi^2}\sqrt{d(s_0)/r(s_0)}$).

Consider now corrections relating to the non-separability of variables, which causes interchannel scattering. Using a left-coming wave in the nth channel as an initial condition for the iteration procedure

$$C_m^0 = \left(\delta_{nm}/\sqrt{k_n(s)}\right)\exp\left(i\int^s ds' \, k_n(s')\right)$$

one obtains from (3) for the reflection coefficient ($n \neq m$)

$$R_{nm} = \left|\int_{-\infty}^{+\infty} \frac{ds}{2\sqrt{k_n k_m}} V_{nm} \exp\left(i\int^s ds' \, (k_n + k_m)\right)\right|^2.$$

Under the assumptions made, transmission and reflection coefficients obey the current conservation law in the form $\sum_m T_{nm} = 1 - \sum_m R_{nm}$. According to the WKB approximation, the width $d(s)$ is assumed to vary essentially on the scale

$L > 1/k_n$. If the radius of curvature does not vary faster than the width, then using the asymptotic limit for an integral of a quickly oscillating function one can obtain the following estimate for the reflection coefficient

$$R_{nm} \leqslant \frac{k^4 L^2}{k_n k_m} \left(\frac{d}{r}\right)^2 \exp\left(-2L(k_n + k_m)\right)$$

where both n and m correspond to the channels where an electron undergoes above-barrier reflection ($k_{n,m} \neq 0$). A more detailed analysis of solutions of equation (2), which are analogous to the one given in [8], shows that all other corrections are also exponentially small for a constriction with smooth enough boundaries.

In conclusion, a novel approach is presented which gives a simple criterion for accurate conductance quantization in a constriction of arbitrary shape. The criterion is that at any point of the constriction the width must be much smaller than the radius of curvature of the boundaries. This condition can easily be satisfied even far from the narrowest part of the constriction. In a system satisfying the criterion, an electron wave propagates through the entire device without mode mixing, and the switching on of new channels of propagation is sharp. This provides not only accurate conductance quantization in the plateau region, but also sharp changes from one plateau to the next.

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