Journal of Experimental and Theoretical Physics, Vol. 92, No. 5, 2001, pp. 811–815.
From Zhurnal Éksperimental'noĭ i Teoreticheskoĭ Fiziki, Vol. 119, No. 5, 2001, pp. 931–936.

SOLIDS
Electronic Properties

Conductance of the Elliptically Shaped Quantum Wire¶

S. N. Shevchenko* and Yu. A. Kolesnichenko

Verkin Institute for Low Temperature Physics and Engineering, National Academy of Sciences of Ukraine, Kharkov, 61164 Ukraine
**e-mail: sshevchenko@ilt.kharkov.ua*

Received 25 October, 2000

Abstract—The conductance of a ballistic elliptically shaped quantum wire is investigated theoretically. It is shown that the effect of the curvature results in a strongly oscillating dependence of the conductance on the applied bias. © *2001 MAIK "Nauka/Interperiodica".*

1. INTRODUCTION

Recent advances in semiconductor physics and technology enabled the fabrication and investigation of nanostructure devices possessing important properties, such as small size, reduced dimensionality, relatively small density of charge carriers, and hence, large mean free path (which means that particles exist in the ballistic regime and the scattering processes can therefore be neglected), and large Fermi wavelength λ_F. One of the mesoscopic systems of particular interest is the quantum wire in which particles are constrained to move along a one-dimensional curve due to quantization of the transverse modes.[1] One of the numerous important problems pertaining to the quantum wire is to determine the influence of the reduced dimensionality upon the system properties.

Jensen and Koppe [1] and da Costa [2] emphasized that a low-dimensional system, in general, has some knowledge of the surrounding three-dimensional Cartesian space: the effective potential arises from the mesoscopic confinement process, which constrains particles to move in a domain of a reduced dimensionality. Namely, it was shown that a particle moving in a one- or two-dimensional domain is affected by an attractive effective potential [2]; this result was first obtained in [3] and later in [4]. This idea was widely studied by several other authors (see [5–12] and, for example, [13] about the experimental realization of such systems).

It was also shown in [14] that the torsion of the twisted waveguide affects the wave propagation in the waveguide independently of the nature of the wave. In particular, the torsion of the waveguide results in the rotation of the polarization of light in a twisted optical fiber [15]. In [16], the authors prove that in a waveguide, be it quantum or electromagnetic one, bound states exist. Several papers have been devoted to the relation of the quantum waveguide theory to the classical theory of acoustic and electromagnetic waveguides in [6].

The effect of the curvature on quantum properties of electrons on a two-dimensional surface, in a quantum waveguide, or in a quantum wire can be observed by investigating kinetic and thermodynamic characteristics of quantum systems [8–12]. In this paper, we propose to use measurements of the conductance G of a quantum wire for this purpose; we show that the reflection of electrons from regions with a variable curvature results in a nonmonotonic dependence of the conductance on the applied bias.

In [4], the Schrödinger equation on the elliptically shaped ring was solved numerically in order to obtain the eigenvalue spectrum of a particle confined to the ring. The authors studied a quantum mechanical system confined to a narrow ring by the rectangular well potential. They showed that in the limit as the ring width γ tends to zero, the behavior of the system is similar to the straight line motion with the effective potential

$$V_{\text{eff}} = -\frac{\hbar^2}{8mR^2}, \tag{1}$$

where R is the radius of curvature. Later [9], the electron energy spectrum in an elliptical quantum ring was considered in connection with the persistent current; the authors have concluded that the effective potentials V_{eff} are different for different confining potentials even in the limit as γ tends to zero. This conclusion is in contradiction with the results of some other papers [2, 6]. We address this problem in the present paper; we investigate the derivation of the one-dimensional Schrödinger equation in order to understand more deeply how the particle motion along the curve C is affected by the confining potential. We demonstrate the consistency with the previous results in [2]: the effective potential is universal for different confining potentials and depends only on the curvature (see Eq. (1)).

¶ This article was submitted by the authors in English.

1 We study here only the one-channel wire with only the lowest subband occupied.

1063-7761/01/9205-0811$21.00 © 2001 MAIK "Nauka/Interperiodica"

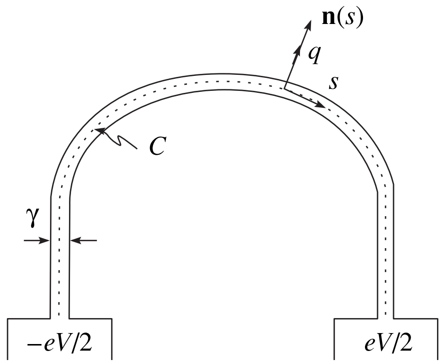

Fig. 1. Elliptically shaped quantum wire.

In Section 2, we derive a one-dimensional Schrödinger equation starting from the two-dimensional Schrödinger equation describing a nonrelativistic electron that moves in a plane[2] and is subjected to the confining potential V_γ. In Section 3, we apply these results to theoretically study the conductance of the quantum wire that consists of two linear parts and one elliptically shaped part between them; the wire is connected to two conducting reservoirs at different voltages (see Fig. 1). In Section 4, we discuss the influence of the curvature on the conductance.

2. SCHRÖDINGER EQUATION

In this section, we follow the approach proposed in [2]. We consider the electron with the effective mass m moving in a quantum wire along a curve C that is constructed by a prior confinement potential V_γ. For simplicity, we start with the two-dimensional motion. We introduce the orthonormal coordinate system[3] (s, q), where s is the arc length parameter and q is the coordinate along the normal $\mathbf{n} = \mathbf{n}(s)$ to the reference curve C. The curve C is then described by a vector valued function $\mathbf{r}(s)$ of the arc length s. In a vicinity of C, the position is therefore described by

$$\mathbf{R}(s, q) = \mathbf{r}(s) + q\mathbf{n}(s). \qquad (2)$$

To obtain a meaningful result, the particle wave function must be "uniformly compressed" into a curve, thereby avoiding tangential forces [2, 4, 9]. We thus consider V_γ to depend only on the q coordinate that describes the displacement from the reference curve C; this means that points with the same q coordinate but different s coordinates (which describe the position on C) have the same potential. This potential involves a small parameter γ such that the potential increases sharply for every small displacement in the normal direction; γ is the characteristic width of the potential well V_γ. The simplest examples of these potentials are the rectangular well potential and the parabolic-trough potential (we note that the real potential would likely be a combination of both, however). The small parameter in the problem is therefore $\gamma/R \ll 1$ [5].

The motion of the electron obeys the time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\Delta_{s,q}\psi + V_\gamma(q)\psi = \varepsilon\psi, \qquad (3)$$

where the Laplacian is

$$\Delta_{s,q} = \frac{1}{h}\frac{\partial}{\partial s}\frac{1}{h}\frac{\partial}{\partial s} + \frac{1}{h}\frac{\partial}{\partial q}h\frac{\partial}{\partial q}, \qquad (4)$$

with

$$h = 1 - k(s)q \qquad (5)$$

being the Lamé coefficient (corresponding to the longitudinal coordinate s) that depends on the curvature $k = k(s)$ in accordance with the Frenet equation.

To eliminate the first-order derivative with respect to q from Eq. (3),[4] we introduce the new wave function $\tilde{\psi}$ by

$$\tilde{\psi}(s, q) = \sqrt{h}\psi(s, q). \qquad (6)$$

This is the wave function introduced in [2] and normalized so that

$$\int ds\, dq |\tilde{\psi}(s, q)|^2 = 1. \qquad (7)$$

The Schrödinger equation (3) then becomes

$$-\frac{\hbar^2}{2m}\left(\frac{\partial}{\partial s}\frac{1}{h^2}\frac{\partial}{\partial s} + \frac{\partial^2}{\partial q^2}\right)\tilde{\psi} + V_{\rm eff}(s, q)\tilde{\psi} + V_\gamma(q)\tilde{\psi} = \varepsilon\tilde{\psi}, \qquad (8)$$

where

$$V_{\rm eff}(s, q) = -\frac{\hbar^2}{2m} \times\left(h^{-2}\frac{k^2}{4} + \frac{q}{2}h^{-2}\frac{d^2k}{ds^2} + \frac{5q^2}{4}h^{-4}\left(\frac{dk}{ds}\right)^2\right), \qquad (9)$$

which is in agreement with [5, 8].

One must be careful with Eq. (8) in order to avoid mistakes found in the literature [7, 9]. First, we cannot decompose this equation, which contains terms that are

[2] We consider only flat curves and we refer the reader interested in the effect of the torsion to [7].

[3] The advantages of establishing the (s, q) coordinate system from the very beginning are that it allows the most general analysis and that (because of the diagonal structure of the metric tensor) we can decompose the dynamical equation of motion into two equations in the zero-order approximation in the width of the quantum wire.

[4] We do this to eliminate terms of the form $f(q)\partial/\partial q$ that were called "dangerous terms" in [1]. We cannot use $f(q) = f(0)$ because $f(q)\partial/\partial q \approx [f(0) + qdf(0)/dq]\partial/\partial q$: although $q \sim \gamma$, we have $\partial/\partial q \sim \gamma^{-1}$ and the second term in the brackets is therefore $\sim\gamma^0$, and this is the order of terms in which we are interested below.

functions of both s and q, into two equations introducing $\tilde{\psi}(s, q) = \chi_n(q)\chi_t(s)$ as in [7], where the authors obtained Eq. (31) for $\chi_t(s)$ with coefficients depending on the q variable. To understand another mistake [9], we consider Eq. (8) within the perturbation theory in the small parameter γ (which is small compared to R) (see also [6]). We expand h^{-2} and V_{eff} in series in $q \lesssim \gamma$ and explicitly write the zeroth term as

$$h^{-2} = 1 + \sum_{l=1}^{\infty} f_l(s) q^l,$$

$$V_{\text{eff}}(s, q) = -\frac{\hbar^2}{2m}\left(\frac{k^2(s)}{4} + \sum_{l=1}^{\infty} y_l(s) q^l\right).$$

Equation (8) can then be rewritten as

$$(\hat{H}_0 + \hat{V})\tilde{\psi} = \varepsilon\tilde{\psi}, \tag{10}$$

where

$$\hat{H}_0 = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial s^2} + \frac{\partial^2}{\partial q^2}\right) - \frac{\hbar^2}{2m}\frac{k^2(s)}{4} + V_\gamma(q), \tag{11}$$

$$\hat{V} = \frac{\hbar^2}{2m}\sum_{l=1}^{\infty} q^l\left(-\frac{\partial}{\partial s} f_l(s)\frac{\partial}{\partial s} + y_l(s)\right). \tag{12}$$

We note that $\hat{V}$ is a second order differential operator in s. The solution of Eq. (10) is

$$\tilde{\psi} = \tilde{\psi}^{(0)} + \sum_{l=1}^{\infty} \tilde{\psi}^{(l)},$$

where $\tilde{\psi}^{(l)} \sim \gamma^l$ and $\tilde{\psi}^{(0)}$ corresponds to the zeroth-order problem, $\hat{H}_0\tilde{\psi}^{(0)} = \varepsilon\tilde{\psi}^{(0)}$. This equation can be decomposed by separating the wave function as $\tilde{\psi}(s, q) = \eta(q)\chi(s)$,

$$-\frac{\hbar^2}{2m}\frac{d^2}{dq^2}\eta + V_\gamma(q)\eta = E_t\eta \tag{13}$$

and

$$-\frac{\hbar^2}{2m}\frac{d^2}{ds^2}\chi + V_{\text{eff}}(s)\chi = E_t\chi, \tag{14}$$

where $V_{\text{eff}}(s)$ is given by Eq. (1), $\varepsilon = E_t + E_l$, and $R = k(s)^{-1}$ is the curvature radius (in the next section, we omit the subscript "l", identifying the energy E with its longitudinal component E_l). Equation (13) describes the confinement of the electron to a γ-neighborhood of the curve C and Eq. (14) describes the motion along the s coordinate (along C). In fact, Eq. (14) is a conventional one-dimensional Schrödinger equation for the electron moving in the s-dependent potential $V_{\text{eff}}(s)$; the latter relates the geometry and the dynamical equation. The origin of this potential is in the wavelike properties of the particles; V_{eff} is essential for the values of R/λ_F that are not large. We emphasize that the effective potential in Eq. (1) in the zeroth-order approximation in γ/R is independent of the "one-dimensionalization" method, i.e., of the choice of $V_\gamma(q)$ (compare this conclusion with the one derived in [9])

We also note that if we started from the three-dimensional equation of motion, we would obtain an additional effective potential that vanishes in the planar situation [2].

3. CONDUCTANCE

The conductance G of quantum contacts can be related to the transmission probability $T(E)$ by Landauer's formula [17]. At zero temperature and finite voltages V, it takes the form

$$G = \frac{G_0}{2}\left[T\left(E_F + \frac{eV}{2}\right) + T\left(E_F - \frac{eV}{2}\right)\right], \tag{15}$$

where $G_0 = 2e^2/h$ and E_F is the Fermi energy. The two terms in this equation correspond to two electronic beams moving in opposite directions with different bias energies. We are interested in the transmission probability $T(E)$ for the electron energy E.

In this section, we consider the curve C to consist of three ideally connected parts (see Fig. 1): (i) linear ($s < 0$), (ii) elliptical ($0 < s < l$, where l is half of the ellipse perimeter), and (iii) one more linear domain ($s > l$). We consider wave functions in regions (i) and (iii) to be the respective plane waves $\psi_1 = e^{ik_1 s} + re^{-ik_1 s}$ and $\psi_3 = te^{ik_1 s}$, where $k_1 = \sqrt{2mE/\hbar^2}$ is the wave vector and t and r are the transmission and reflection coefficients; the transmission probability is given by $T = |t|^2$. We have $\psi_2 \equiv \chi$, where χ is the solution of Eq. (14) with the effective potential given by Eq. (1). The curvature can be written most simply in the elliptical coordinate v [18] defined by its Lamé coefficient

$$H = \frac{ds}{dv} = a\sqrt{1 - e^2\cos^2 v}, \tag{16}$$

where e is the eccentricity of the ellipse and a is the length of its major semiaxis; we use $v(s = 0) = 0$. The effective (geometrical) potential in Eq. (1) can then be written as

$$V_{\text{eff}}(s) = -\frac{\hbar^2}{8ma^2}\frac{1 - e^2}{(1 - e^2\cos^2 v)^3}, \tag{17}$$

which is in agreement with [4].

We introduce the new wave function

$$\xi(v(s)) = \chi(s)/\sqrt{H}, \tag{18}$$

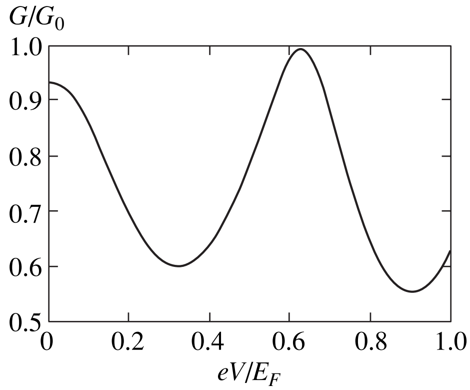

Fig. 2. Conductance as a function of the bias $G = G(eV)$ at $e = 0.99$, $a = 10\lambda_F$ (at the same value of a but with $e = 0$, the amplitude $\Delta G/G_0$ is on the order of 10^{-5}).

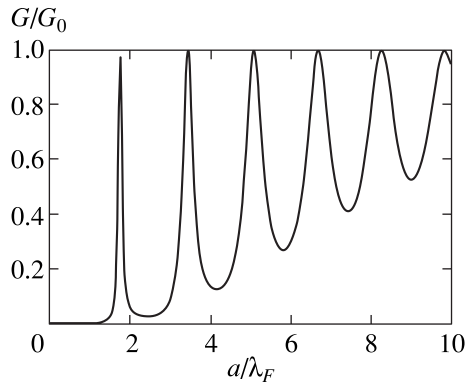

Fig. 3. Conductance as a function of the length of the major semiaxis $G = G(a)$ at $e = 0.99$, $V = 0$.

for which the equation takes the form (see Eqs. (14) and (16)–(18))

$$\frac{d^2}{dv^2}\xi + \left[\frac{2ma^2}{\hbar^2}Eg(v) + U(v)\right]\xi = 0, \quad (19)$$

$$U(v) = \frac{5}{4}\frac{1-e^2}{g^2} - \frac{1-e^2/2}{g} - \frac{e^4}{16}\frac{\sin^2 2v}{g^2}, \quad (20)$$

where $g = H^2/a^2 = 1 - e^2\cos^2 v$. Equation (19) is the Hill equation with π-periodic coefficients; the fundamental system of its solutions is [19]

$$\xi_\pm = e^{\pm i\mu v}y(\pm v), \quad (21)$$

where $y(v)$ is a π-periodic function and μ is the characteristic exponent. We then have (see Eqs. (18) and (21))

$$\chi = C_1 e^{i\mu v}\tilde{y}(v) + C_2 e^{-i\mu v}\tilde{y}(-v), \quad (22)$$

where $\tilde{y}(v) \equiv \sqrt{H}y(v)$.

With the known wave functions, we are now interested in $T = |t|^2$, which describes the transmission over the potential well (see Eq. (17)). We use the continuity conditions for the wave function and its derivative, which gives a system of four equations that is similar to the one given in [20]; the result is

$$T = \left[1 + \frac{1}{4}\left(\kappa - \frac{1}{\kappa}\right)^2 \sin^2\pi\mu\right]^{-1}, \quad (23)$$

where we denoted

$$\kappa = -\frac{i}{ak_1\sqrt{1-e^2}}\left(\frac{\xi_+'}{\xi_+}\right)_{v=0}. \quad (24)$$

(To obtain Eq. (23), we assumed that μ and κ are real, which is straightforward to proof.)

4. RESULTS AND DISCUSSION

To understand how the conductivity G depends on the bias eV and the geometry, we must find the solution of Hill equation (19). We did this numerically and also within the perturbation theory for an ellipse that is close to the circle (i.e., $e^2 \ll 1$); we found that the two solutions are in good agreement for $e < 1/2$. In the zeroth-order approximation in e^2 (i.e., for $e = 0$, the case of a circular arc), we have $\mu_0 = ak_2$ and $\kappa_0 = k_2/k_1$, where $k_2 = \sqrt{2mE/\hbar^2 + 1/4a^2}$ (see also [12]). This implies that oscillations in the $G(V)$ dependence can be observed if $a \gtrsim \lambda_F$ and the amplitude of these oscillations is sufficiently small.

The first-order approximation of the perturbation theory (for $a > \lambda_F$) yields

$$\mu \approx \mu_0 + e^2\mu_1, \quad \kappa \approx \kappa_0 + e^2\kappa_1, \quad (25)$$

where

$$\mu_1 = -\frac{ak_1^2}{4k_2} \equiv \frac{\mu_0}{4\kappa_0^2}, \quad (26)$$

$$\kappa_1 = \frac{k_1}{4k_2((ak_2)^2 - 1)}. \quad (27)$$

We have solved Hill equation (19) numerically. The characteristic exponent μ is defined via the solution of Eq. (19) with the initial conditions $\xi_1(0) = 1$ and $\xi_1'(0) = 0$, and μ is then the solution of the equation $\xi_1(\pi) = \cos\pi\mu$ (see [19]). It is more difficult to find ξ_+ (see Eq. (21)), which can be formulated as the boundary value problem for Eq. (19) with the boundary conditions $\xi_2(0) = 0$ and $\xi_2(\pi) = \sin\pi\mu$ (where $\xi_2(v) = \mathrm{Im}\,\xi_+(v)$). Introducing $\xi_3(v) = \xi_2(v)/\xi_2'(0)$, we have the initial condition problem for $\xi_3(v)$ (with $\xi_3(0) = 0$, and $\xi_3'(0) = 1$), whose solution allows us to define κ, $(\xi_+'/\xi_+)_{v=0} = \xi_2'(0) = \sin\pi\mu/\xi_3(\pi)$. The results of the described procedure are numerically plotted in Figs. 2 and 3 for a sufficiently elongated ellipse with $e = 0.99$

(with $a/b = 7$, where a and b are the respective lengths of its major and minor semiaxes). We note about Fig. 3 that under the restriction $R \gg \gamma$, we must not let a go to zero; namely, we may suppose $R \gg \gamma$ for $a/\lambda_F \sim 10$ but may not for $a/\lambda_F \lesssim 1$ [for e close to unity]. We also note that Eq. (15) is, strictly speaking, correct for eV small compared with E_F and describes $G(V)$ dependence for $eV \sim E_F$ qualitatively. We conclude that e close to unity significantly increases oscillations in comparison to the case of $e = 0$; the amplitude of oscillations in $G = G(V)$ is defined by the value of a/λ_F.

In summary, we have rederived the quantum-mechanical effective potential induced by the curvature of the one-dimensional quantum wire. We have shown that for any confining potential V_γ depending only on the displacement q from the reference curve C, this effective potential is universal: it does not depend on the choice of V_γ and is given by Eq. (1). We have studied the effect of the curvature on the conductance of an ideal elliptically shaped quantum wire in the zeroth-order approximation in the width of the wire. It has been shown, in particular, that due to the effect of the curvature, the dependence of the conductance $G(V)$ on the applied bias changes drastically. Thus, the effect of the curvature can be observed by measuring the conductance of the quantum wire. On the other hand, one can change the characteristics of the quantum wire, such as the conductance, setting its size, shape, or applied bias.

ACKNOWLEDGMENTS

One of the authors (S.N.S.) would like to thank Prof. I.D. Vagner for his warm hospitality during his stay at the Grenoble High Magnetic Field Laboratory (France), where a part of this work was done. We also thank Prof. A.M. Kosevich for critical discussion of the manuscript.

REFERENCES

1. H. Jensen and H. Koppe, Ann. Phys. (N. Y.) **63**, 586 (1971).
2. R. C. T. da Costa, Phys. Rev. A **23**, 1982 (1981).
3. J. Marcus, J. Chem. Phys. **45**, 4493 (1966).
4. E. Switkes, E. L. Russell, and J. L. Skinner, J. Chem. Phys. **67**, 3061 (1977).
5. P. Exner and P. Šeba, J. Math. Phys. **30**, 2574 (1989).
6. P. Duclos and P. Exner, Rev. Math. Phys. **7**, 73 (1995).
7. I. J. Clark and A. J. Bracken, J. Phys. A **29**, 339 (1996).
8. I. J. Clark and A. J. Bracken, J. Phys. A **29**, 4527 (1996).
9. L. I. Magarill, D. A. Romanov, and A. V. Chaplik, Zh. Éksp. Teor. Fiz. **110**, 669 (1996) [JETP **83**, 361 (1996)].
10. L. I. Magarill and A. V. Chaplik, Pis'ma Zh. Éksp. Teor. Fiz. **68**, 136 (1998) [JETP Lett. **68**, 148 (1998)].
11. L. I. Magarill, D. A. Romanov, and A. V. Chaplik, Usp. Fiz. Nauk **170**, 325 (2000).
12. A. Namiranian, M. R. H. Khajehpour, Yu. A. Kolesnichenko, and S. N. Shevchenko, Physica E (Amsterdam) (2001) (in press).
13. V. Ya. Prinz, V. A. Seleznev, V. A. Samoylov, and A. K. Gutakovsky, Microelectron. Eng. **30**, 439 (1996).
14. M. Kugler and S. Shtrikman, Phys. Rev. D **37**, 934 (1988).
15. R. Y. Chiao and Y. S. Wu, Phys. Rev. Lett. **57**, 933 (1986); A. Tomita and R. Y. Chiao, Phys. Rev. Lett. **57**, 937 (1986).
16. J. Goldstone and R. L. Jaffe, Phys. Rev. B **45**, 14100 (1992).
17. R. Landauer, IBM J. Res. Dev. **1**, 233 (1957).
18. E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis* (Cambridge Univ. Press, Cambridge, 1927).
19. E. Kamke, *Differentialgleichungen; Lösungsmethoden und Lösungen* (Geest and Portig, Leipzig, 1959; Nauka, Moscow, 1976).
20. L. D. Landau and E. M. Lifshitz, *Course of Theoretical Physics*, Vol. 3: *Quantum Mechanics: Non-Relativistic Theory* (Nauka, Moscow, 1963; Pergamon, New York, 1965).