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Effect of curvature on conductance of the quantum wire

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

B.I. Verkin Institute for Low Temperature Physics and Engineering, National Academy of Sciences of Ukraine, 47 Lenin Ave., 61103 Kharkov, Ukraine

Abstract

The effect of the curvature-induced quantum mechanical potential on the conductance of the curved quantum wire is investigated theoretically. We demonstrate that the characteristics of the quantum wire, such as conductance, can be changed setting its size, shape, or applied bias. © 2002 Elsevier Science B.V. All rights reserved.

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It was shown that a low-dimensional system, in general, has some knowledge of its surrounding three-dimensional Cartesian space: the effective potential arises from the mesoscopic confinement process which constrains particles to move in domain of reduced dimensionality [1–4]. Namely, it was shown that a particle moving in a one- or two-dimensional domain is affected by attractive effective potential. This idea was widely studied by several other authors (see Refs. [5–11]).

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 [7–10]. In this paper, we propose to use for this purpose measurements of the conductance G of a quantum wire and we show that the reflection of electrons from regions with variable curvature results in non-monotonous dependence of the conductance on the applied bias.

In Ref. [4] the Schrödinger equation on the elliptically shaped ring was solved numerically in order to get the eigenvalue spectrum of a particle confined to the ring. The authors demonstrated that the behavior of a quantum mechanical system confined by the rectangular well potential to a narrow ring in the limit when its width γ tends to zero is analogous to the straight line motion with effective potential

$$V_{\mathrm{eff}} = -\frac{\hbar^2}{8mR^2}, \qquad (1)$$

where $R = k^{-1}$ is the radius of curvature. Later, in Ref. [8] the electron energy spectrum in an elliptical quantum ring was considered in connection with the persistent current.

We will first briefly overview how the effective curvature-induced potential arise. Further, we apply this results to consider theoretically the conductance of the quantum wire which consists of two linear parts and one elliptically shaped part between them, the wire is connected to two conducting reservoirs at different

* Corresponding author. Institute for Low Temperature Physics and Engineering 16th Dpt., 47 Lenin Ave., 61164 Kharkov, Ukraine. Tel.: +380-572-513-517.

E-mail address: sshevchenko@ilt.kharkov.ua (S.N. Shevchenko).

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voltages. And finally we discuss the influence of the curvature on the conductance.

Let us consider an electron with effective mass m moving in a quantum wire along a curve C which is constructed by a prior confinement potential V_γ. For the sake of simplicity, we start from two-dimensional motion. We introduce the orthonormal coordinate system (s,q), where s is the arc length parameter and q is the coordinate along the normal to the reference curve C.

To obtain a meaningful result the particle wave function should be "uniformly compressed" into a curve, avoiding in this way the tangential forces [2,4,8]. So, we consider V_γ to be dependent only on the q-coordinate which describes the displacement from the reference curve C. This potential contains small parameter γ (which is a characteristic width of the potential well V_γ) so that the potential increases sharply for every small displacement in the normal direction. So, the small parameter of the problem is $\gamma/R \ll 1$ [5].

The motion of the electron obeys the two-dimensional time-independent Schrödinger equation which has the form

$$-\frac{\hbar^2}{2m}\triangle_{s,q}\,\psi + V_\gamma(q)\psi = \varepsilon\psi. \tag{2}$$

Introducing $\tilde{\psi}(s,q) = \sqrt{1-k(s)q}\,\psi(s,q)$ (which is normalized so that $\int \mathrm{d}s\,\mathrm{d}q\,|\tilde{\psi}(s,q)|^2 = 1$), we obtain in the zero approximation in γ/R

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial s^2}+\frac{\partial^2}{\partial q^2}\right) - \frac{\hbar^2}{2m}\frac{k^2(s)}{4} + V_\gamma(q) - \varepsilon\right] \times\tilde{\psi}(s,q) = 0. \tag{3}$$

This equation can be decomposed by separating the wave function $\tilde{\psi}(s,q) = \eta(q)\chi(s)$ into two

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}q^2}\eta + V_\gamma(q)\eta = E_\mathrm{t}\eta, \tag{4}$$

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}s^2}\chi + V_\mathrm{eff}(s)\chi = E_\ell\chi, \tag{5}$$

where $V_\mathrm{eff}(s)$ is given by Eq. (1); $\varepsilon = E_\mathrm{t} + E_\ell$ (in the following we omit the subscript "ℓ", identifying energy E with its longitudinal component E_ℓ). Eq. (4) describes the confinement of the electron to a γ-neighborhood of the curve C and Eq. (5) describes the motion along the s coordinate (along the curve C). In fact, Eq. (5) is a conventional one-dimensional Schrödinger equation for an electron moving in the s-dependent potential $V_\mathrm{eff}(s)$, the latter connects the geometry and the dynamical equation. The origin of this potential is in the wave-like properties of the particles; V_eff is essential for not large R/λ_F. We underline that the effective potential (Eq. (1)), in the zeroth-order approximation in γ/R, is universal for different confining potentials $V_\gamma(q)$ and depends only on the curvature (see also in Refs. [2,10,11]).

The conductance G of quantum contacts can be related to the transmission probability $T(E)$ by Landauer's formula [12]. At zero temperature and finite voltages V it takes the form

$$G = \frac{G_0}{2}\left[T\left(E_\mathrm{F}+\frac{\mathrm{eV}}{2}\right) + T\left(E_\mathrm{F}-\frac{\mathrm{eV}}{2}\right)\right], \tag{6}$$

where $G_0 = 2e^2/h$, E_F is the Fermi energy. Two terms in this equation correspond to two electronic beams moving in opposite directions and differing in bias energy. So, we are interested in the transmission probability $T(E)$ with E being an electron energy.

We consider the curve C to consist of three ideally connected parts: (i) linear ($s<0$), (ii) elliptical ($0<s<l$, l is half of the ellipse's perimeter), and (iii) one more linear domain ($s>l$). We consider wave functions in regions (i) and (iii) to be plane waves $\psi_1 = \mathrm{e}^{\mathrm{i}k_1 s} + r\mathrm{e}^{-\mathrm{i}k_1 s}$, $\psi_3 = t\mathrm{e}^{\mathrm{i}k_1 s}$, 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 $T = |t|^2$. The wave function $\psi_2 \equiv \chi$, where χ is the solution of Eq. (5). The curvature can be written most simply in the elliptical v coordinate, then the effective (geometrical) potential from Eq. (1) can be written as

$$V_\mathrm{eff}(v) = -\frac{\hbar^2}{8ma^2}\frac{1-e^2}{(1-e^2\cos^2 v)^3}, \tag{7}$$

where e is the eccentricity of an ellipse and a is the length of its major semiaxis.

We introduce new wave function $\xi(v) = \chi(s(v))/\sqrt{1-e^2\cos^2 v}$ and get the fundamental system of the solutions of Eq. (5) with the potential given by

Eq. (7) (which is the Hill's equation) [13]:

$$\xi_{\pm} = \mathrm{e}^{\pm \mathrm{i}\mu v} y(\pm v), \tag{8}$$

where $y(v)$ is a π-periodic function, and μ is the characteristic exponent.

Then we make use of the conditions of continuity of the wave function and of its derivative, and the result is Ref. [14]

$$T = \left[1 + \frac{1}{4}\left(\kappa - \frac{1}{\kappa}\right)^2 \sin^2 \pi\mu\right]^{-1}, \tag{9}$$

where we denoted

$$\kappa = -\frac{\mathrm{i}}{ak_1\sqrt{1-e^2}}\left(\frac{\xi'_+}{\xi_+}\right)_{v=0}. \tag{10}$$

Then we solve Hill's equation Eq. (5) with potential (7) numerically in order to get the real parameters μ and κ, which we put in Eqs. (9) and (6). And the numerical analysis shows the strongly oscillating dependence of the conductance on both the applied bias eV and the ring size a for the elongated enough ellipses $(1 - e \ll 1)$ [10]. For some values of eV and a conductance becomes equal to G_0, which corresponds to the resonant transmission over the potential well [14]. We also note that the amplitude of oscillations in $G = G(V)$ dependence is defined by the value of a/λ_{F}.

In summary, we have studied the effect of the curvature, in the zeroth-order approximation in the width of the wire, on the conductance of an ideal elliptically shaped quantum wire. It has been explained, in particular, that, due to the effect of the curvature, dependence of the conductance $G(V)$ on the applied bias changes drastically. So, the effect of the curvature can be observed by measuring the conductance of a quantum wire. On the other hand, one can change the characteristics of the quantum wire, such as conductance, setting its size, shape, or applied bias.

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