BEND-IMITATING THEORY AND ELECTRON SCATTERING IN SHARPLY-BENT QUANTUM NANOWIRES

O.O. VAKHNENKO

Bogolyubov Institute for Theoretical Physics, Nat. Acad. of Sci. of Ukraine
(14-B, Metrologichna Street, Kyïv 03143, Ukraine; e-mail: vakhnenko@bitp.kiev.ua)

PACS 73.21.Hb, 61.46.Km, 03.65.Nk

The concept of bend-imitating description as applied to the one-electron quantum mechanics in sharply-bent ideal electron waveguides and its development into a self-consistent theory are presented. In general, the theory allows one to model each particular circular-like bend of a continuous quantum wire as some specific multichannel scatterer being point-like in the longitudinal direction. In an equivalent formulation, the theory gives rise to rather simple matching rules for the electron wave function and its longitudinal derivative affecting only the straight parts of a wire and thereby permitting one to bypass a detailed quantum mechanical consideration of elbow domains. The proposed technique is applicable to the analytical investigation of spectral and transport properties related to the ideal sharply-bent 3D wire-like structures of fixed cross-section and is adaptable to the 2D wire-like structures, as well as to the wire-like structures in the magnetic field perpendicular to the wire bending plane.

In the framework of bend-imitating approach, the investigation of the electron scattering in a doubly-bent 2D quantum wire with S-like bend has been made, and the explicit dependences of the transmission and reflection coefficients on geometrical parameters of a structure, as well as on the electron energy, have been obtained.

The total elimination of the mixing between the scattering channels of a S-like bent quantum wire is predicted.

1. Introduction

The experimental discovery of the conductance quantization exhibited by two-dimensional Sharvin contacts [1, 2] and two-dimensional nanowires [3] in the ballistic regime is known to get unleashed a flood of investigations devoted to the spectral and transport properties of wire-like nanostructures [4–36]. The term "ballistic regime" means that the maximal typical size of a nanostructure must be much smaller than the transport mean free path of an electron. As long as the condition of ballisticity is fulfilled, we may expect that, inside the nanostructure, neither the temperature effects nor the effects of electron interactions are relevant, and, therefore, the electron behavior can be treated quantum-mechanically presumably in the one-electron approximation. However, in order that the quantum effects be probed both experimentally and theoretically, the minimal width of a nanostructure must exceed the de Broglie wavelength corresponding to the typical Fermi energy of an electron in macroscopic reservoirs connected to the nanostructure. Here, the reservoirs and the nanostructure are regarded as having the same operating dimensionality with respect to the electron degrees of freedom.

Due to its definition, the ballistic regime should provide the spectral and transport characteristics of a probed nanostructure with features of the purely geometric origin [4–23, 31–36], thereby prompting the idea of creating the required nanoscale device through solely the choice of a proper geometric configuration. There are numerous attempts to come out beyond the framework of ballistic consideration, e.g., taking the impact of impurities or other imperfections into account [24–29] or trying to approximate the charging effects [30], but we discard such an attitude insofar, as there still exist many interesting and nontrivial problems attributed to the ideal (i.e. quantum) nanostructures albeit treatable within the traditional quantum mechanics.

In this paper, we will deal with the bent quantum wires of a fixed cross-section, thus relinquishing other types of nanostructures (i.e. crossed wires [10–14, 27] and wires of a variable cross-section [15–25, 29]) irre-

spective to their perfectness. More precisely, by starting from the one-electron quantum mechanics, we will give a detailed development of the bend-imitating theory [31, 32] allowing one to identify the bent parts of a sharply-bent quantum wire with some effective scatterers, each being shrunken to zero in the longitudinal direction. We will demonstrate the calculating power of the bent-imitating technique by an example of the electron scattering in two-dimensional sharply-bent quantum wires. Early, the advantages of the bent-imitating approach had been thoroughly examined when studying the localized electronic states [31, 32] which are certain to arise as a generic consequence of the wire bending [5, 33, 34], as well as when proposing the effect of resonant electronic transmission in multiple-bent quantum nanowires of some special configurations [31].

2. Specification of the Wire Bending in Terms of Orthogonal Curvilinear Coordinates

The first natural step in considering the quantum mechanics of an electron in a bent ideal wire with fixed cross-section is to adapt the orthogonal curvilinear coordinates to the shape of a wire. Having been classical in the theories of diffraction [37] and guided propagation of electromagnetic waves [38], as well as in the theory of guided propagation of light through optical fibers [39], the idea of curvilinear coordinates lately have been invoked by the theory of bent nanowires [31–36].

In our papers on the electron scattering in smoothly-bent quantum wires [35, 36], we have proposed a specific parametrization of the wire bending which turned out to be essentially more productive when being properly applied to the one-electron quantum-mechanical problems in the opposite limit of sharply-bent wires [31, 32].

To make the story shorter, the metric tensor components $g_{\rho\rho}(\rho, s, z)$, $g_{ss}(\rho, s, z)$, and $g_{zz}(\rho, s, z)$ in orthogonal curvilinear coordinates ρ, s, z dictated by the wire bending must be given in the following way:

$$g_{\rho\rho}(\rho, s, z) = 1, \tag{2.1}$$

$$g_{ss}(\rho, s, z) = [1 + a(s/L)\rho/L]^2, \tag{2.2}$$

$$g_{zz}(\rho, s, z) = 1. \tag{2.3}$$

Here, $a(s/L)$ is the so-called bending function [35, 36] characterizing the wire bending through the bending angle 2β and the typical bending length L of the reference curve $y = f(x)$ given in terms of orthogonal Cartesian coordinates x, y in the plane $z = 0$. In this context, the reference function

$$f(x) = L \tan\beta \, \mathrm{arsinh}[\cot\beta \, \cosh(x/L)] \tag{2.4}$$

leads uniquely to the bending function

$$a(s/L) = \frac{\sin\beta \, \cos^2\beta}{\sinh^2[(s/L)\cos\beta] + \cos^2\beta}\,. \tag{2.5}$$

The above statement can be easily checked excluding the auxiliary parameter η from the general geometric relations [35, 36]

$$a(s/L) = \frac{Ld^2 f(\eta)/d\eta^2}{[1 + (df(\eta)/d\eta)^2]^{3/2}}, \tag{2.6}$$

$$s = \int\limits_0^\eta d\xi [1 + (df(\xi)/d\xi)^2]^{1/2}, \tag{2.7}$$

where the function $f(\eta)$ is assumed to be concave $d^2 f(\eta)/d\eta^2 > 0$ at all values $-\infty < \eta < +\infty$ of its argument η. Analyzing the asymptotics $-x\tan\beta + L\tan\beta\ln(\cot\beta)$ and $+x\tan\beta + L\tan\beta\ln(\cot\beta)$ of the chosen reference function (2.4) at $x/L \to -\infty$ and $x/L \to +\infty$, we can readily recognize the early announced bending parameters in 2β and L.

It is worth noting that the simultaneous representability of both the reference function $f(x)$ and the corresponding bending function $a(s/L)$ in terms of elementary functions as it has been displayed by formulas (2.4) and (2.5) seems to be rather the lucky exception than an established rule. In the dilemma which function, $f(x)$ or $a(s/L)$, should be taken as elementary, the preference casts onto the bending function $a(s/L)$ as that directly involved into the metric tensor and consequently into the Laplace operator in the curvilinear coordinates of interest. Evidently, we are able to invent a number of bending functions whose reference curves manifest the essential similarity in their asymptotic features and differ only by minor peculiarities within the bending regions. For example, instead of the infinity-pole bending function (2.5), it is possible to rely upon the two-pole bending function [31, 32]

$$a(s/L) = \frac{2\beta/\pi}{(s/L)^2 + 1}, \tag{2.8}$$

inasmuch as it preserves the interpretation of the basic parameters 2β and L as the bending angle and the bending length, respectively.

Supposing the central point of each cross-section of a wire to lie in the plane $z = 0$ and denoting d to be a typical width of the wire in this plane, we define the dimensionless longitudinal coordinate σ by the formula $s = \sigma d$. Then the dimensionless parameter $\varepsilon = d/L$ will characterize the sharpness of wire bending with $\varepsilon \ll 1$ and $\varepsilon \gg 1$ corresponding to the smooth and the sharp bending, respectively. Furthermore at $\varepsilon \to \infty$, we afford the reference curve to be converted into two straight half-lines interconnected practically at a single point, while each particular coordinate line of constant positive ρ to be degenerated into two straight lines interconnected by the circular arc of radius ρ and angle 2β. In this very limit, the two forms (2.5) and (2.8) of a bending function $a(s/L)$ become indistinguishable insofar as

$$\lim_{\varepsilon\to\infty} \varepsilon a(\varepsilon\sigma) = 2\beta\delta(\sigma) \tag{2.9}$$

for both of them. Here, $\delta(\sigma)$ is the Dirac delta-function. The latter observation (2.9) turned out to be the main cornerstone in an upbuilding of the bend-imitating theory [31, 32].

Considering that the quantity $\sqrt{g_{ss}(\rho, s, z)} = 1 + a(s/L)\rho/L$ determines the whole structure of the Laplace operator, we must deal with the confining potential, which totally prohibits the electron penetration into the region $\rho \leqslant -L/a(s/L)$, where the curvilinear coordinates ρ, s, z become generically ambiguous. The most radical way in achieving such a prohibition is to ensure that the wire edges should be located somewhere in the region $\rho \geqslant 0$. For the lucidity, we would like to stress that the line $\rho = 0$, $z = 0$ is nothing but the reference curve written in terms of the adopted curvilinear coordinates.

3. Three-dimensional and Two-dimensional Bend-imitating Models

In the previous sections, we have mentioned all assumptions and made the main preparatory steps necessary to formulate the one-electron quantum mechanics for an arbitrary bent ideal wire with fixed cross-section. Thus, relating the curvilinear coordinates ρ, s, z and time t to their dimensionless counterparts r, σ, ζ, and τ by the formulas $\rho = rd$, $s = \sigma d$, $z = \zeta d$, and $t = 2m^*d^2\tau/\hbar$, we can write down the respective Schrödinger equation as follows:

$$i\frac{\partial}{\partial\tau}\Psi(r,\sigma,\zeta,\tau) =$$

$$= -[1+\varepsilon ra(\varepsilon\sigma)]^{-1}\frac{\partial}{\partial r}\left\{[1+\varepsilon ra(\varepsilon\sigma)]\frac{\partial}{\partial r}\Psi(r,\sigma,\zeta,\tau)\right\} -$$

$$-[1+\varepsilon ra(\varepsilon\sigma)]^{-1}\frac{\partial}{\partial\sigma}\left\{[1+\varepsilon ra(\varepsilon\sigma)]^{-1}\frac{\partial}{\partial\sigma}\Psi(r,\sigma,\zeta,\tau)\right\} -$$

$$-\frac{\partial^2}{\partial\zeta^2}\Psi(r,\sigma,\zeta,\tau) + W(r,\zeta)\Psi(r,\sigma,\zeta,\tau), \tag{3.1}$$

where the early suggested notations (2.1)–(2.3) for the components of the metric tensor have been taken into account. In so doing, m^* is the effective electron mass, while the expression $(\hbar^2/2m^*d^2)W(\rho/d, z/d)$ has the meaning of lateral confining potential caused by the wire walls. According to their definitions, the coordinates ρ and z vary across the wire, while the coordinate s runs along the wire. In this respect, the dimensionless coordinates r and ζ should be referred to as the lateral ones, while the dimensionless coordinate σ as the longitudinal one.

Until the explicit expression for the bending function $a(\varepsilon\sigma)$ was not specified, the Schrödinger equation (3.1) looks rather general and virtually contains nothing new as compared with the standard starting position of other curvilinear coordinate approaches [33, 34]. However, multiplying the original Schrödinger equation (3.1) by the Jacobian $1 + \varepsilon ra(\varepsilon\sigma)$ and rearranging the result into the form

$$\left[i\frac{\partial}{\partial\tau} + \frac{\partial^2}{\partial r^2} + \frac{\partial^2}{\partial\sigma^2} + \frac{\partial^2}{\partial\zeta^2} - W(r,\zeta)\right]\Psi(r,\sigma,\zeta,\tau) =$$

$$= -\varepsilon ra(\varepsilon\sigma)\left[i\frac{\partial}{\partial\tau} + \frac{\partial^2}{\partial\zeta^2} - W(r,\zeta)\right]\Psi(r,\sigma,\zeta,\tau) -$$

$$-\varepsilon a(\varepsilon\sigma)\frac{\partial}{\partial r}\left[r\frac{\partial}{\partial r}\Psi(r,\sigma,\zeta,\tau)\right] +$$

$$+\frac{\partial}{\partial\sigma}\left[\frac{\varepsilon ra(\varepsilon\sigma)}{1+\varepsilon ra(\varepsilon\sigma)}\frac{\partial}{\partial\sigma}\Psi(r,\sigma,\zeta,\tau)\right], \tag{3.2}$$

we can readily reveal the crucial hint on future simplifications in the limit of sharp bending $\varepsilon \to \infty$, once the special expression (2.5) or (2.8) for the bending function $a(\varepsilon\sigma)$ has been invoked. This hint concerns the first two terms on the right-hand side of the rearranged equation (3.2), where the factor $\varepsilon a(\varepsilon\sigma)$ should be formally replaced by its limiting value $2\beta\delta(\sigma)$ in virtue of the main limiting property (2.9).

As for the last term on the right-hand side of the rearranged equation (3.2), the direct passage to the limit $\varepsilon \to \infty$ in it appears to be impractical due to the unproper behavior of the quantity $\partial\{\varepsilon ra(\varepsilon\sigma)[1+\varepsilon ra(\varepsilon\sigma)]^{-1}\}/\partial\sigma$ as a function of σ (s.s. the extremal values of this function become unbounded as $\varepsilon \to \infty$). However, the quantity $\varepsilon ra(\varepsilon\sigma)[1+\varepsilon ra(\varepsilon\sigma)]^{-1}$ as a function of

σ is seen to be bounded at all permissible ε including $\varepsilon \to \infty$. Moreover, both $\partial\{\varepsilon ra(\varepsilon\sigma)[1+\varepsilon ra(\varepsilon\sigma)]^{-1}\}/\partial\sigma$ and $\varepsilon ra(\varepsilon\sigma)[1+\varepsilon ra(\varepsilon\sigma)]^{-1}$ quickly drop to zero, as $|\sigma|$ grows, what become highly pronounced for the extremely sharp bending $\varepsilon \to \infty$. In these circumstances, it is reasonable to abandon the detailed description of the bent area and to develop the matching procedure for a wave function directly between the straightened parts of a wire akin to the well-known matching procedure in quantum-mechanical problems with delta-function-like potentials [40].

To this end, we apply the operation $\lim_{\gamma\to+0}\lim_{\varepsilon\to\infty}\int_{-\gamma}^{+\gamma} d\sigma\ldots$ to the rearranged equation (3.2) and obtain

$$\frac{\partial}{\partial\sigma}\Psi(r,\sigma=-0,\zeta,\tau)-\frac{\partial}{\partial\sigma}\Psi(r,\sigma=+0,\zeta,\tau)=$$
$$=\beta r\left[i\frac{\partial}{\partial\tau}+\frac{\partial^2}{\partial\zeta^2}-W(r,\zeta)\right]\Psi(r,\sigma=-0,\zeta,\tau)+$$
$$+\beta r\left[i\frac{\partial}{\partial\tau}+\frac{\partial^2}{\partial\zeta^2}-W(r,\zeta)\right]\Psi(r,\sigma=+0,\zeta,\tau)+$$
$$+\beta\frac{\partial}{\partial r}\left[r\frac{\partial}{\partial r}\Psi(r,\sigma=-0,\zeta,\tau)\right]+$$
$$+\beta\frac{\partial}{\partial r}\left[r\frac{\partial}{\partial r}\Psi(r,\sigma=+0,\zeta,\tau)\right]. \tag{3.3}$$

Here and later on, any record of the type $\partial\Upsilon(\sigma=\lambda)/\partial\sigma$ serves as a shorthand for the expression $[\partial\Upsilon(\sigma)/\partial\sigma]_{\sigma=\lambda}$. On the other hand, applying the operation $\lim_{\gamma\to+0}\lim_{\varepsilon\to\infty}\int_{-\gamma}^{+\gamma} d\sigma\sigma\ldots$ to the same equation (3.2), we have

$$\Psi(r,\sigma=-0,\zeta,\tau)=\Psi(r,\sigma=+0,\zeta,\tau). \tag{3.4}$$

In both cases, we assumed that the passage to the limit $\varepsilon\to\infty$ is performed before that to the limit $\gamma\to+0$. Thus, we come to the bend-imitating matching rules (3.3) and (3.4) which should supplement the Schrödinger equation

$$i\frac{\partial}{\partial\tau}\Psi(r,\sigma,\zeta,\tau)=$$
$$=\left[-\frac{\partial^2}{\partial r^2}-\frac{\partial^2}{\partial\sigma^2}-\frac{\partial^2}{\partial\zeta^2}+W(r,\zeta)\right]\Psi(r,\sigma,\zeta,\tau)$$
$$(\sigma\neq 0) \tag{3.5}$$

given in the straight parts of the wire $|\sigma|>0$, thus yielding a closed formulation of the one-electron quantum mechanics outside the bending area. This formulation can be referred to as the bend-imitating model of a quantum wire with fixed cross-section of an arbitrary configuration and with the ring arc bend characterized by the angle 2β.

It is remarkable that the last term on the right-hand side of the rearranged equation (3.2) does not contribute to either of the matching rules (3.3) and (3.4). As a consequence, it is possible to give an alternative concise formulation of the bend-imitating model by means of a single equation

$$\left[i\frac{\partial}{\partial\tau}+\frac{\partial^2}{\partial r^2}+\frac{\partial^2}{\partial\sigma^2}+\frac{\partial^2}{\partial\zeta^2}-W(r,\zeta)\right]\Psi(r,\sigma,\zeta,\tau)=$$
$$=-2\beta\delta(\sigma)r\left[i\frac{\partial}{\partial\tau}+\frac{\partial^2}{\partial\zeta^2}-W(r,\zeta)\right]\Psi(r,\sigma,\zeta,\tau)-$$
$$-2\beta\delta(\sigma)\frac{\partial}{\partial r}\left[r\frac{\partial}{\partial r}\Psi(r,\sigma,\zeta,\tau)\right]. \tag{3.6}$$

Irrespective of the model formulation, the values of confining potential taken at $r\leqslant 0$ must be infinite, i.e. $W(r\leqslant 0,\zeta)=\infty$.

If we intend to consider a wire with circular cross-section, it is convenient to introduce the polar lateral coordinates u and θ instead of the coordinates r and ζ by the rules

$$r=b+u\cos\varphi, \tag{3.7}$$

$$\zeta=u\sin\varphi \tag{3.8}$$

with $u\geqslant 0$ and $0\leqslant\varphi<2\pi$, where b is the dimensionless distance between the reference curve and the center of a wire. Then, denoting

$$\Psi(b+u\cos\varphi,\sigma,u\sin\varphi,\tau)=\Phi(\sigma,u,\varphi,\tau) \tag{3.9}$$

and

$$W(b+u\cos\varphi,u\sin\varphi)=V(u,\varphi), \tag{3.10}$$

we are able to convert the basic bend-imitating model (3.6) into the form

$$\left[i\frac{\partial}{\partial\tau}+\frac{\partial^2}{\partial\sigma^2}+\frac{\partial^2}{\partial u^2}+\frac{1}{u}\frac{\partial}{\partial u}+\frac{1}{u^2}\frac{\partial^2}{\partial\varphi^2}-V(u,\varphi)\right]\Phi(\sigma,u,\varphi,\tau)=$$
$$=-2\beta\delta(\sigma)\left[\cos\varphi\frac{\partial}{\partial u}-\frac{\sin\varphi}{u}\frac{\partial}{\partial\varphi}\right]\Phi(\sigma,u,\varphi,\tau)-$$
$$-2\beta\delta(\sigma)[b+u\cos\varphi]\times$$
$$\times\left[i\frac{\partial}{\partial\tau}+\frac{\partial^2}{\partial u^2}+\frac{1}{u}\frac{\partial}{\partial u}+\frac{1}{u^2}\frac{\partial^2}{\partial\varphi^2}-V(u,\varphi)\right]\Phi(\sigma,u,\varphi,\tau). \tag{3.11}$$

In order to guarantee the general demand $W(r \leqslant 0, \zeta) = \infty$, it is appropriate to assume that $V(u \geqslant b, \varphi) = \infty$.

A generalization of the bend-imitating model as applied to a multiply-bent multiply-twisted quantum wire with circular cross-section in the case where $V(u, \varphi) \equiv V(u)$ had been given elsewhere [31].

Another particular realization of the bend-imitating theory concerns the so-called two-dimensional quantum wires. The reduced dimensionality is known to be approximately achieved in an interface of GaAs–$Al_xGa_{1-x}As$ heterostructure [41, 42] while the 2D wire itself can be stencilled by applying the negative potential of a certain configuration, thus expelling electrons from the prescribed parts of the interface [43–45]. The approximate two-dimensionality of the electron gas is caused by a huge separation between the electron energy levels corresponding to the extremely strong confinement of electrons within the interface layer, so that only the lowest of such levels is actually became essential.

In view of the above remark, the derivation of a bend-imitating model of sharply-bent 2D quantum wire can be reduced to the formal factorization

$$\Psi(r, \sigma, \zeta, \tau) = \psi(r, \sigma, \tau)\chi(\zeta, \tau) \tag{3.12}$$

of the wave function $\Psi(r, \sigma, \zeta, \tau)$ involved into the basic 3D bend-imitating model (3.6) with additive confinement potential

$$W(r, \zeta) = U(r) + V(\zeta). \tag{3.13}$$

These steps ensure that, in a direction perpendicular to the interface, the Schrödinger equation

$$\left[i\frac{\partial}{\partial\tau} + \frac{\partial^2}{\partial\zeta^2} - V(\zeta)\right]\chi(\zeta, \tau) = 0 \tag{3.14}$$

can be separated, while the result for the 2D bend-imitating model of singly-bent quantum wire is as follows:

$$\left[i\frac{\partial}{\partial\tau} + \frac{\partial^2}{\partial r^2} + \frac{\partial^2}{\partial\sigma^2} - U(r)\right]\psi(r, \sigma, \tau) =$$
$$= -2\beta r\delta(\sigma)\left[i\frac{\partial}{\partial\tau} - U(r)\right]\psi(r, \sigma, \tau) -$$
$$-2\beta\delta(\sigma)\frac{\partial}{\partial r}\left[r\frac{\partial}{\partial r}\psi(r, \sigma, \tau)\right]. \tag{3.15}$$

We complete this section by presenting the bend-imitating model of 2D quantum wire in a magnetic field $\boldsymbol{B}$ perpendicular to the plane of a wire. When developing such a model, the starting Schrödinger equation must be properly changed via replacing the Laplace operator $\Delta \equiv \nabla^2$ by the operator $(\nabla - ie\boldsymbol{A}/c\hbar)^2$ and supplementing the lateral confinement potential by the Zeeman term $-e\hbar B/2m^*c$ or $+e\hbar B/2m^*c$ with the sign $-$ or $+$ being dictated by the sign $+$ or $-$ of the spin projection onto the vector $\boldsymbol{B}$. Here, the magnetic field intensity $\boldsymbol{B}$ is related to the vector potential $\boldsymbol{A}$ by the usual definition $\boldsymbol{B} = \mathrm{rot}\boldsymbol{A}$, while $e \equiv -|e|$ denotes the electron charge. Relying upon the curvilinear coordinates ρ, s, z, as they have been introduced in Section 2, it is convenient to select the vector potential

$$\boldsymbol{A}(\rho, s, z) = A_\rho(\rho, s, z)\boldsymbol{\iota}_\rho(\rho, s) +$$
$$+A_s(\rho, s, z)\boldsymbol{\iota}_s(\rho, s) + A_z(\rho, s, z)\boldsymbol{\iota}_z(\rho, s) \tag{3.16}$$

in the following gauge

$$A_\rho(\rho, s, z) = 0, \tag{3.17}$$

$$A_s(\rho, s, z) = B\frac{(\rho - \delta)L + \rho^2 a(s/L)/2}{L + \rho a(s/L)}, \tag{3.18}$$

$$A_z(\rho, s, z) = 0. \tag{3.19}$$

Here, δ is the gauge parameter measurable in length units. Although the quantity δ could be chosen as any function of the longitudinal coordinate s, but we shall identify it with the distance bd between the reference curve $\rho = 0$ and the middle line of a wire $\rho = bd$.

Repeating the main steps of the derivation procedure early approbated for the basic 3D bend-imitating model (3.6) and considering the standard reduction procedure from a three-dimensional to a two-dimensional wire, we come to the following formulation of the bend-imitating model dealing with a 2D quantum wire in the perpendicular magnetic field:

$$\left\{i\frac{\partial}{\partial\tau} + \frac{\partial^2}{\partial r^2} + \left[\frac{\partial}{\partial\sigma} - i\omega(r - b)\right]^2 \pm\omega - U(r)\right\}\psi_\pm(r, \sigma, \tau) =$$
$$= -2\beta r\delta(\sigma)\left[i\frac{\partial}{\partial\tau} - \frac{\omega^2 r^2}{4} \pm \omega - U(r)\right]\psi_\pm(r, \sigma, \tau) -$$
$$-2\beta\delta(\sigma)\frac{\partial}{\partial r}\left[r\frac{\partial}{\partial r}\psi_\pm(r, \sigma, \tau)\right] \tag{3.20}$$

Here, the upper and lower signs in $\psi_\pm(r, \sigma, \tau)$ and $\pm\omega$ are used to distinguish two possible electron subsystems according to the sigh of a spin projection. The quantity $\omega = ed^2B/c\hbar$ characterizes the strength of the applied magnetic field given in dimensionless units. The generalization of the above-presented bend-imitating model (3.20) to the case of a multiply-bent 2D quantum wire in

a perpendicular magnetic field can be done in lines with the results of our previous article [32]. The simplest way to visualize such a generalization is to take the dimensionless Zeeman term $\mp\omega$ into account by adding it formally to the dimensionless confinement potential on both sides of Eq. (8) from the cited paper [32]. In doing so, we must pay an especial attention to that the origin of the lateral coordinate in the just quoted formula is fastened to the middle line of a wire in distinction to formula (3.20) from the present paper, where the origin of the lateral coordinate lies on the reference curve.

4. Electron Scattering in a Sharply-bend 2D Quantum Wire. General Setting of the Problem

Now, let us consider the stationary scattering problem of electron waves in a sharply-bent 2D quantum wire starting with the respective concise formulation of one-electron quantum mechanics (3.15).

We denote the dimensionless distance between the reference curve $r = 0$ and the middle line of a wire as b and assume the lateral confinement to be given by the dimensionless hard-wall potential

$$U(r) = \begin{cases} 0 & \text{if} \quad |r-b| < 1/2 \\ \infty & \text{if} \quad |r-b| \geqslant 1/2 \end{cases} \tag{4.1}$$

with the condition $b \geqslant 1/2$ being imposed. For practical use, it is convenient to introduce the shifted lateral coordinate

$$r' = r - b \tag{4.2}$$

with $r' = 0$ and $r' = -b$ marking the middle line of a wire and the reference curve, respectively. Simultaneously, we have to reset the confining potential by the notation

$$U(r'+b) \equiv \mathscr{U}(r') \tag{4.3}$$

and make the substitution

$$\psi(r'+b, \sigma, \tau) = \psi(r', \sigma)\exp(-i\mathscr{E}\tau) \tag{4.4}$$

consistent with the nomenclature of stationary scattering theory. Then, after some manipulations with the concise form (3.15) of the 2D bend-imitating model, we obtain

$$\left[-\frac{\partial^2}{\partial r^2} - \frac{\partial^2}{\partial \sigma^2} + \mathscr{U}(r)\right]\psi(r,\sigma) = \mathscr{E}\psi(r,\sigma) \quad (\sigma \neq 0), \tag{4.5}$$

$$\frac{\partial}{\partial\sigma}\psi(r,\sigma=-0) - \frac{\partial}{\partial\sigma}\psi(r,\sigma=+0) =$$
$$= \beta(r+b)[\mathscr{E} - \mathscr{U}(r)][\psi(r,\sigma=-0) + \psi(r,\sigma=+0)] +$$
$$+\beta\frac{\partial}{\partial r}\Big[(r+b)\frac{\partial}{\partial r}\psi(r,\sigma=-0)\Big] +$$
$$+\beta\frac{\partial}{\partial r}\Big[(r+b)\frac{\partial}{\partial r}\psi(r,\sigma=+0)\Big], \tag{4.6}$$

$$\psi(r,\sigma=-0) = \psi(r,\sigma=+0), \tag{4.7}$$

where $\mathscr{E}$ serves as the dimensionless electron energy. The prime $'$ near the shifted lateral coordinate r' in the last three formulas (4.5)–(4.7) has been omitted as quite useless.

We clearly see that the effect of electron scattering should be entirely obliged to the bent part of a wire modeled by the matching rules (4.7) and (4.6) for the stationary wave function $\psi(r,\sigma)$ and its longitudinal derivative $\partial\psi(r,\sigma)/\partial\sigma$. As for the stationary Schrödinger equation in straight regions (4.5), its role is reduced to the sole approbation of suitable scattering ansätze for the wave function outside the bent area $|\sigma| > 0$.

For our purposes, such ansätze must be given by the combinations

$$\psi(r,\sigma) = Q_f(r)\exp[+iq_f(\mathscr{E})\sigma]H\big(q_f^2(\mathscr{E})\big) +$$
$$+\sum_{m=1}^{\infty} Q_m(r)\exp[-iq_m(\mathscr{E})\sigma]A_{mf}(\mathscr{E},\beta,b) \tag{4.8}$$

and

$$\psi(r,\sigma) = \sum_{m=1}^{\infty} Q_m(r)\exp[+iq_m(\mathscr{E})\sigma]B_{mf}(\mathscr{E},\beta,b) \tag{4.9}$$

at $\sigma < 0$ and $\sigma > 0$, respectively. Here,

$$H(x) = \begin{cases} 1 & \text{if} \quad x \geqslant 0 \\ 0 & \text{if} \quad x < 0 \end{cases} \tag{4.10}$$

is the Heaviside step function,

$$q_m(\mathscr{E}) = \begin{cases} \sqrt{\mathscr{E} - \mathscr{E}_m^{\perp}} & \text{if} \quad \mathscr{E} \geqslant \mathscr{E}_m^{\perp} \\ i\sqrt{\mathscr{E}_m^{\perp} - \mathscr{E}} & \text{if} \quad \mathscr{E} < \mathscr{E}_m^{\perp}, \end{cases} \tag{4.11}$$

while

$$\mathscr{E}_m^{\perp} = (\pi m)^2 \tag{4.12}$$

and

$$Q_m(r) = \begin{cases} \sqrt{2}\sin[\pi m(r+1/2)] & \text{if} \quad |r| \leqslant 1/2 \\ 0 & \text{if} \quad |r| > 1/2 \end{cases} \tag{4.13}$$

are, respectively, the eigenvalues and the orthonormal eigenfunctions of the lateral eigenvalue problem

$$-\frac{d^2}{dr^2}\,Q(r)+\mathscr{U}(r)Q(r)=\mathscr{E}^{\perp}Q(r). \tag{4.14}$$

The ordinal number m in formulas (4.11)–(4.13) can run from one to infinity: $m=1,2,3,\ldots,\infty$.

The first term on the right-hand side of the first ansatz (4.8) describes the ingoing electron wave, while the other terms in both ansätze (4.8) and (4.9) correspond to outgoing waves if $q_m^2(\mathscr{E})\geqslant 0$ or evanescent solutions if $q_m^2(\mathscr{E})<0$. As a matter of fact, the adopted ansätze (4.8) and (4.9) manifest an essential similarity with those typical of multichannel scattering theory [46]. Hence, the scattering theory in sharply-bent quantum wire must be treated in the general case as the multichannel one with the m-th scattering channel being attributed to the m-th electronic level of lateral quantization. In lines with the standard terminology [46], the m-th channel should be referred to as open when $q_m^2(\mathscr{E})\geqslant 0$ and closed otherwise (i.e., when $q_m^2(\mathscr{E})<0$).

By construction, we can understand the first and the second ansätze (4.8) and (4.9) as the two complementary pieces of the same wave function $\psi(r,\sigma)$ satisfying in the straight parts of a wire to the same stationary Schrödinger equation (4.5). The only problem which has to be handled is to find the amplitudes $A_{mf}(\mathscr{E},\beta,b)$ and $B_{mf}(\mathscr{E},\beta,b)$ involved into the above-mentioned ansätze (4.8) and (4.9). To this end, we insert expressions (4.8) and (4.9) into the bend-imitating matching rules (4.6) and (4.7) and obtain

$$q_n(\mathscr{E})A_{nf}(\mathscr{E},\beta,b)=i\beta b\sum_{m=1}^{\infty}M_{nm}(\mathscr{E}|b)B_{mf}(\mathscr{E},\beta,b), \tag{4.15}$$

$$B_{nf}(\mathscr{E},\beta,b)=\delta_{nf}H\big(q_f^2(\mathscr{E})\big)+A_{nf}(\mathscr{E},\beta,b), \tag{4.16}$$

where the matrix elements $M_{nm}(\mathscr{E}|b)$ are given by the formula

$$M_{nm}(\mathscr{E}|b)=q_n^2(\mathscr{E})\delta_{nm}-\big[q_n^2(\mathscr{E})+q_m^2(\mathscr{E})\big]\times$$
$$\times\frac{4nm(1-\delta_{nm})}{b(n+m)^2(\pi n-\pi m)^2}\sin^2\left(\frac{\pi n-\pi m}{2}\right). \tag{4.17}$$

Evidently, these elements are symmetric under the index permutation $M_{nm}(\mathscr{E}|b)=M_{mn}(\mathscr{E}|b)$, simultaneously being purely real $M_{nm}^{*}(\mathscr{E}|b)=M_{nm}(\mathscr{E}|b)$. Depending on whether the indices n and m are equal, $n=m$, or distinct, $n\neq m$, the matrix elements $M_{nm}(\mathscr{E}|b)$ should be qualified as supporting either the self-action within a particular scattering channel or the channel-channel mixing between the channels of opposite parities. As for the distinct channels of the same parity, they are seen to remain unmixed. The product $2\beta b$ determines the length of the mean line within the ring arc sector of a wire, thus serving as the main governing parameter of electron scattering on the strength of the first algebraic bend-imitating matching equation (4.15).

Now it is time to present some rigorous results regarding the bend-imitating theory without any reference to a particular choice of the scattering length $2\beta b$. First of all, one can readily verify that the bend-imitating matching conditions written in their original form (4.6) and (4.7) are compatible with the conservation law of electronic flux through the bent area

$$\int\limits_{-1/2}^{+1/2}dr\left[\psi(r,\sigma)\frac{\partial}{\partial\sigma}\,\psi^{*}(r,\sigma)-\psi^{*}(r,\sigma)\frac{\partial}{\partial\sigma}\,\psi(r,\sigma)\right]_{\sigma=-0}=$$
$$=\int\limits_{-1/2}^{+1/2}dr\left[\psi(r,\sigma)\frac{\partial}{\partial\sigma}\,\psi^{*}(r,\sigma)-\psi^{*}(r,\sigma)\frac{\partial}{\partial\sigma}\,\psi(r,\sigma)\right]_{\sigma=+0} \tag{4.18}$$

i.e. convert the above equality (4.18) into the sheer identity. In the wake of this important observation, the inserting of the left-piece (4.8) and right-piece (4.9) ansätze for the stationary wave function $\psi(r,\sigma)$ into the law of flux conservation (4.18) gives rise to the formula

$$\sum_{m=1}^{\infty}\big[q_m^{*}(\mathscr{E})+q_m(\mathscr{E})\big]\,A_{mf}(\mathscr{E},\beta,b)A_{mf}^{*}(\mathscr{E},\beta,b)+$$
$$+\sum_{m=1}^{\infty}\big[q_m^{*}(\mathscr{E})+q_m(\mathscr{E})\big]\,B_{mf}(\mathscr{E},\beta,b)B_{mf}^{*}(\mathscr{E},\beta,b)=$$
$$=\big[q_f^{*}(\mathscr{E})+q_f(\mathscr{E})\big]\,H\big(q_f^2(\mathscr{E})\big)H^{*}\big(q_f^2(\mathscr{E})\big) \tag{4.19}$$

allowing to introduce the transmission

$$T_{mf}(\mathscr{E},\beta,b)=\frac{q_m(\mathscr{E})}{q_f(\mathscr{E})}B_{mf}(\mathscr{E},\beta,b)B_{mf}^{*}(\mathscr{E},\beta,b) \tag{4.20}$$

and reflection

$$R_{mf}(\mathscr{E},\beta,b)=\frac{q_m(\mathscr{E})}{q_f(\mathscr{E})}A_{mf}(\mathscr{E},\beta,b)A_{mf}^{*}(\mathscr{E},\beta,b) \tag{4.21}$$

coefficients for the channels with $q_m^2(\mathscr{E})\geqslant 0$, i.e. for the open channels. The total number of open channels $N(\mathscr{E})$ depends on the electron energy $\mathscr{E}$ and is determined by

the formula

$$N(\mathscr{E}) = \sum_{m=1}^{\infty} H\big(q_m^2(\mathscr{E})\big). \qquad (4.22)$$

Thus, definitions (4.20) and (4.21) for the transmission $T_{mf}(\mathscr{E},\beta,b)$ and reflection $R_{mf}(\mathscr{E},\beta,b)$ coefficients are valid provided $m \leqslant N(\mathscr{E})$. On account of the condition $q_m^2(\mathscr{E}) < 0$ specifying the closed channels and maintaining the equality $q_m(\mathscr{E}) + q_m^*(\mathscr{E}) = 0$, expressions (4.20) and (4.21) for the transmission and reflection coefficients permit us to rewrite constraint (4.19) on the amplitudes $A_{mf}(\mathscr{E},\beta,b)$ and $B_{mf}(\mathscr{E},\beta,b)$ as the sum rule

$$\sum_{m=1}^{N(\mathscr{E})} [T_{mf}(\mathscr{E},\beta,b) + R_{mf}(\mathscr{E},\beta,b)] = H\big(q_f^2(\mathscr{E})\big) \qquad (4.23)$$

typical of the multichannel scattering theory.

There are at least two approaches to the solution of the infinite sets of linear algebraic equations (4.15) and (4.16) serving as the algebraic matching equations for the amplitudes $A_{mf}(\mathscr{E},\beta,b)$ and $B_{mf}(\mathscr{E},\beta,b)$ and, hence, to the calculation of the transmission $T_{mf}(\mathscr{E},\beta,b)$ and reflection $R_{mf}(\mathscr{E},\beta,b)$ coefficients, being the basic characteristics of electron scattering due to the wire bending.

The first approach can be applied in two extreme cases of small $\beta b \ll 1$ and large $\beta b \gg 1$ scattering distances, when it is possible to seek the solutions to the algebraic matching equations (4.15) and (4.16) by expanding the amplitudes $A_{mf}(\mathscr{E},\beta,b)$ and $B_{mf}(\mathscr{E},\beta,b)$ in the appropriate power series. Although this method gives the explicit dependences of the scattering characteristics $T_{mf}(\mathscr{E},\beta,b)$ and $R_{mf}(\mathscr{E},\beta,b)$ on the geometric parameters β, b and the energy $\mathscr{E}$, it suffers from the irregularity with respect to the energy $\mathscr{E}$ and should be abandoned when the energy $\mathscr{E}$ approaches any energy $(\pi n)^2$ of the lateral quantization.

The second approach is capable to cover the entire feasible energy interval and consists in the so-called N-channel approximation. The idea of the N-channel approximation is rather simple and is based upon replacing the infinite sets of linear algebraic equations (4.15) and (4.16) with $n = 1, 2, 3, \ldots, \infty$ by the respective finite sets with $n = 1, 2, 3, \ldots, N$ provided each summation over m being restricted by first N terms. Here, the positive integer N must exceed the maximal admissible number of open scattering channels $N(\mathscr{E}_{\max})$ within the energy interval $\pi^2 \leqslant \mathscr{E} \leqslant \mathscr{E}_{\max}$ chosen for investigation. Once the maximal number of open channels $N(\mathscr{E}_{\max})$ has been fixed, the accuracy of the N-channel approximation increases, as the number N grows. In this situation, it looks more reasonable to invoke the support of computer simulations. However, we shall postpone a practical realization of this plan due to the lack of knowledge in computer science.

Instead, we would like to pay attention on a broad class of sharply-bent wire-like structures, where all calculations in the framework of the bend-imitating approach can be performed analytically without any further approximations. The simplest and simultaneously basic specimen of this class is an S-like sharply-bent 3D quantum wire with rectangular cross-section or equally well an S-like sharply-bent 2D quantum wire.

The scattering properties of an S-like sharply-bent 2D quantum wire will be studied in the next section.

5. Electron Scattering in S-like Sharply-bent 2D Quantum Wire. Suppression of Mixing between the Scattering Channels

Let us consider the ideal 2D wire-like structure consisting of two half-infinite parts. The left part is supposed to be a sharply-bent quantum wire possessing the concave bending. The right part is supposed to be a sharply-bent quantum wire possessing the convex bending. Then combining two different bend-imitating schemes, having been originated separately from the left and right parts of a structure, into the single scheme, we are able to formulate the unified bend-imitating treatment of one-electron quantum mechanics for the doubly-bent 2D wire-like structure as a whole.

In its stationary version, the unified model looks as follows:

$$\left[-\frac{\partial^2}{\partial r^2} - \frac{\partial^2}{\partial \sigma^2} + \mathscr{U}(r)\right]\psi(r,\sigma) = \mathscr{E}\psi(r,\sigma) \quad (|\sigma| \neq \lambda), \qquad (5.1)$$

$$\begin{aligned}
&\frac{\partial}{\partial\sigma}\psi(r,\sigma=-\lambda-0) - \frac{\partial}{\partial\sigma}\psi(r,\sigma=-\lambda+0) = \\
&= \beta_{\mathrm{L}}\big(b_{\mathrm{L}}+r\big)[\mathscr{E} - \mathscr{U}(r)] \times \\
&\times[\psi(r,\sigma=-\lambda-0) + \psi(r,\sigma=-\lambda+0)] + \\
&+\beta_{\mathrm{L}}\frac{\partial}{\partial r}\Big[\big(b_{\mathrm{L}}+r\big)\frac{\partial}{\partial r}\psi(r,\sigma=-\lambda-0)\Big] + \\
&+\beta_{\mathrm{L}}\frac{\partial}{\partial r}\Big[\big(b_{\mathrm{L}}+r\big)\frac{\partial}{\partial r}\psi(r,\sigma=-\lambda+0)\Big],
\end{aligned} \qquad (5.2)$$

$$\psi(r,\sigma=-\lambda-0) = \psi(r,\sigma=-\lambda+0), \qquad (5.3)$$

$$\frac{\partial}{\partial\sigma}\psi(r,\sigma=+\lambda-0)-\frac{\partial}{\partial\sigma}\psi(r,\sigma=+\lambda+0)=$$
$$=\beta_{\rm R}\big(b_{\rm R}-r\big)[\mathscr{E}-\mathscr{U}(r)]\times$$
$$\times[\psi(r,\sigma=+\lambda-0)+\psi(r,\sigma=+\lambda+0)]+$$
$$+\beta_{\rm R}\frac{\partial}{\partial r}\Big[\big(b_{\rm R}-r\big)\frac{\partial}{\partial r}\psi(r,\sigma=+\lambda-0)\Big]+$$
$$+\beta_{\rm R}\frac{\partial}{\partial r}\Big[\big(b_{\rm R}-r\big)\frac{\partial}{\partial r}\psi(r,\sigma=+\lambda+0)\Big], \quad (5.4)$$

$$\psi(r,\sigma=+\lambda-0)=\psi(r,\sigma=+\lambda+0). \quad (5.5)$$

Here, $2\beta_{\rm L}$ and $2\beta_{\rm R}$ are the bending angles of the left and right elbow domains, respectively, whereas $b_{\rm L}$ and $b_{\rm R}$ are their dimensionless mean bending radii. The quantity 2λ defines the dimensionless distance between the elbow domains.

In order to define the S-like sharply-bent structure, we must equalize the bending angles $\beta_{\rm L}=\alpha=\beta_{\rm R}$ and assume that the dimensionless distance 2λ is negligibly small $\lambda=+0$. Within these assumptions, the previous model (5.1) – (5.5) is reduced to the Schrödinger equation

$$\left[-\frac{\partial^2}{\partial r^2}-\frac{\partial^2}{\partial\sigma^2}+\mathscr{U}(r)\right]\psi(r,\sigma)=\mathscr{E}\psi(r,\sigma)\quad(|\sigma|>0) \quad (5.6)$$

associated with two half-infinite straight parts of a wire and to two exceptionally simple matching rules

$$\frac{\partial}{\partial\sigma}\psi(r,\sigma=-0)-\frac{\partial}{\partial\sigma}\psi(r,\sigma=+0)=$$
$$=\alpha c\left[\mathscr{E}+\frac{\partial^2}{\partial r^2}-\mathscr{U}(r)\right]\psi(r,\sigma=-0)+$$
$$+\alpha c\left[\mathscr{E}+\frac{\partial^2}{\partial r^2}-\mathscr{U}(r)\right]\psi(r,\sigma=+0), \quad (5.7)$$

$$\psi(r,\sigma=-0)=\psi(r,\sigma=+0) \quad (5.8)$$

serving to imitate the S-like bending area. Here, the notation $c\equiv b_{\rm L}+b_{\rm R}$ has been adopted so that the quantity $2\alpha c$ can be understood as the total dimensionless scattering length.

It is remarkable that, due to the S-like geometry of a wire bending, the matching rule (5.7) for the longitudinal derivative of the one-electron wave function has lost the terms responsible for the mixing of scattering channels. As a consequence, the scattering problem in an S-like sharply-bent 2D quantum wire simplifies to the easy exercise.

Indeed, seeking the solution in the form

$$\psi(r,\sigma)=Q_f(r)\exp\big[+iq_f(\mathscr{E})\sigma\big]H\big(q_f^2(\mathscr{E})\big)+$$
$$+\sum_{m=1}^{\infty}Q_m(r)\exp\big[-iq_m(\mathscr{E})\sigma\big]A_{mf}(\mathscr{E},\alpha c)$$
$$(\sigma<0), \quad (5.9)$$

$$\psi(r,\sigma)=\sum_{m=1}^{\infty}Q_m(r)\exp\big[+iq_m(\mathscr{E})\sigma\big]B_{mf}(\mathscr{E},\alpha c)$$
$$(\sigma>0) \quad (5.10)$$

satisfying to the Schrödinger equation (5.6), we come, by virtue of the matching rules (5.7) and (5.8), to the set of only two linear algebraic equations

$$A_{nf}(\mathscr{E},\alpha c)=i\alpha cq_n(\mathscr{E})B_{nf}(\mathscr{E},\alpha c), \quad (5.11)$$

$$B_{nf}(\mathscr{E},\alpha c)=\delta_{nf}H\big(q_f^2(\mathscr{E})\big)+A_{nf}(\mathscr{E},\alpha c), \quad (5.12)$$

where the ordinal number of the scattering channel n albeit running from one to infinity appears as the mere parameter. According to these equations, the solutions for the amplitudes $A_{nf}(\mathscr{E},\alpha c)$ and $B_{nf}(\mathscr{E},\alpha c)$ read

$$A_{nf}(\mathscr{E},\alpha c)=\frac{i\alpha cq_n(\mathscr{E})\delta_{nf}H(q_f^2(\mathscr{E}))}{1-i\alpha cq_n(\mathscr{E})}, \quad (5.13)$$

$$B_{nf}(\mathscr{E},\alpha c)=\frac{\delta_{nf}H(q_f^2(\mathscr{E}))}{1-i\alpha cq_n(\mathscr{E})}\ . \quad (5.14)$$

Then, for the transmission $T_{nf}(\mathscr{E},\alpha c)$ and reflection $R_{nf}(\mathscr{E},\alpha c)$ coefficients, we obtain

$$T_{nf}(\mathscr{E},\alpha c)=\frac{q_n(\mathscr{E})}{q_f(\mathscr{E})}B_{nf}(\mathscr{E},\alpha c)B^*_{nf}(\mathscr{E},\alpha c)=$$
$$=\frac{\delta_{nf}H(q_f^2(\mathscr{E}))}{1+\alpha^2c^2q_f^2(\mathscr{E})}, \quad (5.15)$$

$$R_{nf}(\mathscr{E},\alpha c)=\frac{q_n(\mathscr{E})}{q_f(\mathscr{E})}A_{nf}(\mathscr{E},\alpha c)A^*_{nf}(\mathscr{E},\alpha c)=$$
$$=\frac{\alpha^2c^2\delta_{nf}q_f^2(\mathscr{E})H(q_f^2(\mathscr{E}))}{1+\alpha^2c^2q_f^2(\mathscr{E})}\ , \quad (5.16)$$

where $n\leqslant N(\mathscr{E})$. These results are seen to be very transparent for the analysis and exhibit the strict one-channel behavior at all physically admissible values of geometric and energetic parameters $2\alpha c$ and $\mathscr{E}$.

6. Conclusion

Summarizing the main results of the paper, we have made the systematic development of the bend-imitating theory rendering the one-electron quantum mechanics to be applied to sharply-bent 2D quantum wires both in the presence and the absence of a perpendicular magnetic field, as well as to sharply-bent 3D quantum wires of any fixed cross-section including the circular one. In the framework of this theory, each elbow domain of a wire is modeled by some attractive multichannel scatterer, being point-like in the longitudinal direction. In an alternative but equivalent formulation, the theory allows one to consider the Schrödinger equation only within the straight regions of a wire and to match the respective solutions directly by means of specific bend-imitating matching rules, thus canceling the cumbersome matching procedure inherent in the traditional approach [5, 7–9], where the solutions within elbow domains had to be involved. As a consequence, the proposed matching technique gives rise to the cardinal simplification of calculations and can be treated as an effective ruse in bypassing each bent part of a wire.

In this context, it can be shown that the bend-imitating matching rules prove to be consistent with the standard continuity equation, where the density is understood as the electron density, as well as with the continuity equation, where the role of density is prescribed to the density of electron energy. These tests assert to be the good general indications of the reliability and the adequacy of the bend-imitating method as such.

Another important general property of the bend-imitating modeling is its consistency with the additivity of bending angles when the longitudinal distance between similarly bent neighboring elbow domains of equal mean radii tends to zero.

It is worth noting that the factual development of the bend-imitating theory had not been so straightforward as it being given in the present article. Thus, the early version of the theory [47–49], though yielding the correct results for the energies of true localized states (i.e. states below the threshold electron energy) suffers to contradict some of the general demands listed in two previous paragraphes.

We have demonstrated the advantages of the bend-imitating approach as applied to the one-electron scattering problem in a doubly-bent 2D quantum wire with S-like bend. The analytical results for the transmission and reflection coefficients as functions of the geometric and energetic parameters have been obtained rigorously, i.e. without any subsequent approximations.

In the framework of the bend-imitating theory, we have shown that, in an S-like bent 2D quantum wire, the mixing of scattering channels is totally eliminated due to a specific interplay between the concave and convex bendings. The same effect is evidently valid for the S-like bent 3D quantum wire with rectangular cross-section. We do not know any indications on the similar forecasting in researches of other authors.

We do not see any principal obstacles in applying the ideas of the bend-imitating theory to the investigation of nonlinear excitations in curved waveguides early studied by other methods [50–52], since the incorporation of a nonlinearity is equivalent to the formal supplement of a confinement potential by the proper nonlinear term.

The work has been supported by the National Academy of Sciences of Ukraine within the programs No. 0110U007540 and No. 0107U000396.

1. B.J. van Wees, H. van Houten, C.W.J. Beenakker, J.G. Williamson, L.P. Kouwenhoven, D. van der Marel, and C.T. Foxon, Phys. Rev. Lett. **60**, 848 (1988).
2. D.A. Wharam, T.J. Thornton, R. Newbury, M. Pepper, H. Ahmed, J.E.F. Frost, D.G. Hasko, D.C. Peacock, D.A. Ritchie, and G.A.C. Jones, J. Phys. C **21**, L209 (1988).
3. J.C. Wu, M.N. Wybourne, W. Yindeepol, A. Weisshaar, and S.M. Goodnick, Appl. Phys. Lett. **59**, 102 (1991).
4. G. Kirczenow, Phys. Rev. B **39**, 10452 (1989).
5. F. Sols and M. Macucci, Phys. Rev. B **41**, 11887 (1990).
6. C.S. Lent, Appl. Phys. Lett. **56**, 2554 (1990).
7. K. Vacek, H. Kasai, and A. Okiji, J. Phys. Soc. Japan **61**, 27 (1992).
8. K. Vacek, A. Okiji, and H. Kasai, Phys. Rev. B **47**, 3695 (1993).
9. K.-F. Berggren and Zhen-Li Ji, Phys. Rev. B **47**, 6390 (1993).
10. R.L. Schult, D.G.Ravenhall, and H.W. Wyld, Phys. Rev. B **39**, 5476 (1989).
11. T. Kakuta, Y. Takagaki, K. Gamo, S. Namba, S. Takaoka, and K. Murase, Phys. Rev. B **43**, 14321 (1991).
12. Y. Takagaki and D.K. Ferry, Phys. Rev. B **44**, 8399 (1991).
13. Yu. B. Gaididei, L.I. Malysheva, and A.I. Onipko, Phys. stat. sol. (b) **172**, 667 (1992).
14. Yu. B. Gaididei, L.I. Malysheva, and A.I. Onipko, J. Phys.: Condens. Matter **4**, 7103 (1992).
15. P. Exner, P. Šeba, and P. Št'oviček, Czech. J. Phys. B **39**, 1181 (1989).
16. C.S. Lent and M. Leng, J. Appl. Phys. **70**, 3157 (1991).

17. K.-F. Berggren and Zhen-Li Ji, Phys. Rev. B **43**, 4760 (1991).
18. Zhen-Li Ji and K.-F. Berggren, Phys. Rev. B **45**, 6652 (1992).
19. H. Wu and D.W.L. Sprung, Phys. Rev. B **47**, 1500 (1993).
20. J.P. Carini, J.T. Londergan, K. Mullen, and D.P. Murdock, Phys. Rev. B **48**, 4503 (1993).
21. Yu. A. Klimenko and A.I. Onipko, Low Temp. Phys. **20**, 721 (1994).
22. M. Andrews and C.M. Savage, Phys. Rev. A **50**, 4535 (1994).
23. M.V. Moskalets, Low Temp. Phys. **23**, 235 (1997).
24. Y. Takagaki and D.K. Ferry, Phys. Rev. B **45**, 6715 (1992).
25. T. Kawamura and J.P. Leburton, Phys. Rev. B **48**, 8857 (1993).
26. Y. Meir and N.S. Wingreen, Phys. Rev. Lett. **68**, 2512 (1992).
27. T. Sakamoto, Y. Takagaki, K. Gamo, S. Namba, S. Takaoka, and K. Murase, Solid State Commun. **80**, 535 (1991).
28. A. Mosk, Th.M. Nieuwenhuizen, and C. Barnes, Phys. Rev. B **53**, 15914 (1996).
29. Y. Takagaki and D.K. Ferry, J. Phys.: Condens. Matter **4**, 10421 (1992).
30. I. Zozulenko, J. Phys.: Condens. Matter **6**, 5507 (1994).
31. O.O. Vakhnenko, Phys. Lett. A **231**, 419 (1997).
32. O.O. Vakhnenko, Phys. Lett. A **249**, 349 (1998).
33. P. Exner and P. Seba, J. Math. Phys. **30**, 2574 (1989).
34. J. Goldstone and R.L. Jaffe, Phys. Rev. B **45**, 14100 (1992).
35. O.O. Vakhnenko and Yu. B. Gaididei, Ukr. Fiz. Zh. **38**, 906 (1993).
36. Yu. B. Gaididei and O.O. Vakhnenko, J. Phys.: Condens. Matter **6**, 3229 (1994).
37. V.M. Babich and V.S. Buldyrev, *Short-Wavelength Diffraction Theory. Asymptotic Methods* (Springer, Berlin, 1991).
38. V.V. Borisov, *Nonstationary Fields in Waveguides* (LGU, Leningrad, 1991) (in Russian).
39. A.K. Hobbs and W.L. Kath, IMA J. Appl. Math. **44**, 197 (1990).
40. S. Flügge, *Practical Quantum Mechanics I* (Springer, Berlin, 1971).
41. F.M. Peeters and O. Hipólito, Brazilian J. Phys. **22**, 183 (1992).
42. S. Datta, *Electronic Transport in Mesoscopic Systems* (Cambridge Univ. Press, Cambridge, 1995).
43. T.J. Thornton, M. Pepper, H. Ahmed, D. Andrews, and G.J. Davies, Phys. Rev. Lett. **56**, 1198 (1986).
44. G. Bernstein and D.K. Ferry, J. Vac. Sci. Technol. B **5**, 964 (1987).
45. A. Shailos, J.P. Bird, M.P. Lilly, J.L. Reno, and J.A. Simmons, J. Phys.: Condens. Matter **18**, 3277 (2006).
46. A.S. Davydov, *Quantum Mechanics* (Pergamon Press, Oxford, 1976)].
47. O.O. Vakhnenko, Ukr. Fiz. Zh. **39**, 745 (1994).
48. O.O. Vakhnenko, Phys. Rev. B **52**, 17386 (1995).
49. O.O. Vakhnenko, Phys. Lett. A **211**, 46 (1996).
50. C. Gorria, Yu.B. Gaididei, M.P. Soerensen, P.L. Christiansen, and J.G. Caputo, Phys. Rev. B **69**, 134506 (2004).
51. Yu.B. Gaididei, P.L. Christiansen, P.G. Kevrekidis, H. Büttner, and A.R. Bishop, New J. Phys. **7**, 52 (2005).
52. Yu.B. Gaididei, Eur. Phys. J. Special Topics **147**, 153 (2007).

ЗГИН-ІМІТАЦІЙНА ТЕОРІЯ ТА РОЗСІЮВАННЯ ЕЛЕКТРОННИХ ХВИЛЬ В РІЗКО ЗІГНУТИХ КВАНТОВИХ НАНОДРОТАХ

О.О. Вахненко

Р е з ю м е

Представлено концепцію згин-імітаційного опису стосовно одноелектронної квантової механіки для різко зігнутих ідеальних електронних хвилеводів та розвинуто її до меж самодостатньої теорії. На загал така теорія дозволяє трактувати кожний окремий скруглений згин неперервного квантового дроту як деякий специфічний багатоканальний розсіювач з нехтовно малим розміром у поздовжньому напрямку. Як наслідок теорія породжує досить прості правила зшивання для електронної хвильової функції та її поздовжньої похідної, тим самим дозволяючи уникнути детального квантово-механічного розгляду областей згину. Згин-імітаційний підхід є потужним аналітичним прийомом для дослідження спектральних і транспортних характеристик як тривимірних, так і двовимірних дротоподібних наноструктур з різкими згинами, включаючи дротоподібні структури, що зазнають впливу магнітного поля, перпендикулярного до площини згину. В рамках згин-імітаційної теорії досліджено розсіювання електронів у подвійно зігнутому двовимірному квантовому дроті з S-подібним згином. Одержано явні аналітичні залежності для коефіцієнтів проходження та відбиття електронних хвиль як від геометричних параметрів, так і від енергії електрона. Теоретично передбачено повну відсутність перемішування між каналами розсіювання в квантовому дроті з S-подібним згином.