PHYSICAL REVIEW B **88**, 165409 (2013)

# Spin sensitive electron transmission through helical potentials

A. A. Eremko[*] and V. M. Loktev[†]
*Bogolyubov Institute for Theoretical Physics of NAS of Ukraine, Kyiv, Ukraine*

(Received 20 June 2013; revised manuscript received 29 August 2013; published 14 October 2013)

We calculate the transmission coefficient for electrons passing through the helically shaped potential barrier which can be, for example, produced by DNA molecules.

DOI: 10.1103/PhysRevB.88.165409 PACS number(s): 72.25.−b, 73.22.−f, 73.63.−b, 87.85.J−

*Introduction*. In the last years, it was discovered that electron transmission through ordered thin films of chiral molecules is highly spin selective.[1–5] This effect was termed the chiral-induced spin selectivity (CISS) effect[4] (for details see the review Ref. 6 and references therein). In experiments,[2,4] the transmission of photoelectrons through self-assembled monolayers (SAMs) of double-stranded DNA (dsDNA) on gold has been studied. The spin polarization (SP) of electrons ejected from Au substrate and transmitted through SAM of dsDNA was measured and the strong SP, which is defined as[4] $P = (I_\uparrow - I_\downarrow)/(I_\uparrow + I_\downarrow)$ was observed. Here $I_\uparrow$ and $I_\downarrow$ are the intensities of the signals corresponding to the SP oriented parallel and antiparallel to the electrons' velocity, respectively.

Recently, different models have been proposed to explain experimental results.[7–10] A scattering theory in the first Born approximation has been applied to obtain the SP in the differential cross section of electrons moving through chiral molecules with energies above the vacuum level.[8] The model of point charges placed along a helical line is considered in a tight-binding approximation for electronic structure of the helix and the transmission of distinct electron spin state is computed by the Landauer formulation.[9] The SP conductance through a metal-DNA-metal structure is calculated in a tight-binding picture.[10] Although all these studies differ in details, they possess a similar physical basis. Each of them is based on accounting of the spin-orbit interaction (SOI) of an electron that is moving through a helical potential. In other words, describing different aspects of the problem, approaches are based on the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\triangle + V - i\frac{\hbar^2}{4m^2c^2}(\boldsymbol{\sigma}\times\nabla V)\cdot\nabla\right]\Psi = E\Psi, \tag{1}$$

which describes electron states in a potential $V \equiv V(\mathbf{r})$. Here $\Psi(\mathbf{r})$ is an electron spinor wave function, $m$ is the electron mass, and the last term in the brackets describes the SOI: $H_{SO} = \lambda(\boldsymbol{\sigma}\times\nabla V)\cdot\mathbf{p}$ which enters into the Hamiltonian from a nonrelativistic approximation to the Dirac equation (see, e.g., Ref. 11). Here $\boldsymbol{\sigma}$ is a vector whose components are the Pauli matrices $\sigma_j$ $(j = x,y,z)$, $\lambda = \hbar/(2mc)^2$, and $\mathbf{p} = -i\hbar\nabla$ is a momentum operator.

In experiments,[2,4] the photoelectrons have an energy above vacuum level as they transmit through the SAM of dsDNA molecules and then to the detector. These experimental results are our main motivation to consider the problem of an electron transmission through the plane-parallel region with the potential $V(\mathbf{r})$ caused by ordered dsDNA molecules in a monolayer. Although our study has common physics with the above papers,[8–10] it differs by the general statement of the problem, and gives complementary features to the SOI role for the CISS. In particular, we calculate analytically continuous energy eigenfunctions of Eq. (1) to obtain the transmission coefficient for electrons passing through the chiral potential barrier.

*Potential with chiral symmetry*. In the space one can, by convention, separate a cylindrical volume with one dsDNA molecule whose axis coincides with a molecule's symmetry axis. There the electrostatic field arises from the charge distribution in a molecule and hence the potential $V(\mathbf{r})$ for external electrons can be written down as $V(\mathbf{r}) = \sum_n V_n(\mathbf{r})$ with $V_n(\mathbf{r}) = \sum_j V_j(|\mathbf{r} - \mathbf{R}_{n,j}|)$ where $\mathbf{R}_{n,j} = (R_0 + \delta_j)\cos(\frac{2\pi}{N_0}n + \phi_j)\mathbf{e}_x + (R_0 + \delta_j)\sin(\frac{2\pi}{N_0}n + \phi_j)\mathbf{e}_y + (\frac{b}{N_0}n + \zeta_j)\mathbf{e}_z$ indicates the position of the $j$th atomic unit in the $n$th repeating cell of a molecule. Here $R_0$ and $b$ are, correspondingly, the radius and the pitch of the right-handed for definiteness helix at which centers of repeating cells $\mathbf{R}_n$ are placed, $N_0$ is the number of cells per one pitch, $\delta_j$, $\phi_j$, and $\zeta_j$ indicate an exact position of $j$th atomic unit in a cell, and unit vectors $\mathbf{e}_x,\mathbf{e}_y,\mathbf{e}_z$ correspond to laboratory coordinate axis directions.

In cylindrical coordinates $(\rho,\varphi,z)$, it is easy to show that $V(\mathbf{r}) = \sum_n V(\rho,\varphi - 2\pi n/N_0, z - bn/N_0)$. This potential is invariant under helical translation defined as the translation along $z$ by the distance $bn/N_0$ with simultaneous rotation around the $z$ axis by angle $2\pi n/N_0$. Under such translation a point with coordinate $(\rho,\varphi,z)$ moves along the helical curve $\mathbf{r}(\tau)$ represented in a parametrized form

$$\rho(\tau) = \rho, \quad \varphi(\tau) = \varphi + 2\pi\tau, \quad z(\tau) = z + b\tau. \tag{2}$$

The potential $V(\mathbf{r})$ is invariant at displacement $\tau = n/N_0$. This means that at moving along the helical curves (2) the potential is periodical, i.e., it is a periodic function of a parametrization parameter $\tau$ with the period $T = 1/N_0$. As any periodic function, it can be represented by the Fourier series

$$V(\mathbf{r}) = \sum_g V_g e^{igl(\varphi,z)}, \tag{3}$$

where

$$l(\varphi,z) = \frac{1}{2}\left(\frac{z}{b} + \frac{\varphi}{2\pi}\right), \quad g = \frac{2\pi}{T}p$$

with $p$ being integer. Along a helical curve (2) the phase $l(\varphi,z)$ varies as $l(\varphi(\tau),z(\tau)) = l(\varphi,z) + \tau$ and $V(\mathbf{r})$ is the periodic

1098-0121/2013/88(16)/165409(5)

function of $\tau$. The Fourier coefficients $V_g$ are determined by the line integral of a scalar field along a helical curve $\mathbf{r}(\tau)$ which is a parametrized by (2):

$$\begin{aligned} V_g &= \frac{1}{T}\int_{\text{(over a period)}} e^{-igl(\varphi,z)}V(\mathbf{r})ds \\ &= N_0 e^{-i[\varphi-(2\pi/b)z](p/2T)} \\ &\quad\times \int_0^T e^{-ig\tau}V\left(\rho,\varphi-\frac{2\pi}{b}z+2\pi\tau,b\tau\right)d\tau. \end{aligned} \tag{4}$$

It is clearly seen that the Fourier coefficients $V_g \equiv V_g(\rho,\varphi,z)$ are characterized by the following dependance on cylindrical coordinates:

$$V_g(\rho,\varphi,z) = V_g\left(\rho,\varphi-\frac{2\pi}{b}z\right), \tag{5}$$

and are invariant under continuous helical translation at which the coordinates are transformed as (2).

Below, considering the electron energy above vacuum level, we will use the nearly free electrons approximation. In this case, as the zero approximation, the oscillating part in (3) can be neglected and zero harmonic $V_0(\rho,\varphi-2\pi z/b)$ is only considered as the potential in Eq. (1).

Because of the potential $V_0(\mathbf{r})$ is invariant under continuous helical translation; the curves (2) are the equipotential lines. Each curve is characterized by a Frenet frame—a moving reference frame of three orthonormal vectors $\mathbf{e}_j$ which describes a curve locally at each point. For the helical curve (2), the Frenet frame is

$$\begin{aligned} \mathbf{e}_t &= -\frac{2\pi\rho}{a(\rho)}\sin\varphi\mathbf{e}_x + \frac{2\pi\rho}{a(\rho)}\cos\varphi\mathbf{e}_y + \frac{b}{a(\rho)}\mathbf{e}_z, \\ \mathbf{e}_b &= \frac{b}{a(\rho)}\sin\varphi\mathbf{e}_x - \frac{b}{a(\rho)}\cos\varphi\mathbf{e}_y + \frac{2\pi\rho}{a(\rho)}\mathbf{e}_z, \\ \mathbf{e}_\rho &= \cos\varphi\mathbf{e}_x + \sin\varphi\mathbf{e}_y, \end{aligned} \tag{6}$$

where $a(\rho)=\sqrt{b^2+(2\pi\rho)^2}$ is the arc length of one turn of the helix of pitch $b$ and radius $\rho$. The orthonormal vectors $\mathbf{e}_t$, $\mathbf{e}_\rho$, and $\mathbf{e}_b$ determine, respectively, the tangent, normal, and binormal directions for the equipotential helical curve at the point $(x,y,z)$.

Calculation $\nabla V_0$ with taking into account (5) and (6) gives $\nabla V_0 = V_\rho\mathbf{e}_\rho + V_b\mathbf{e}_b$, or

$$\nabla V_0 = |\nabla V_0|\mathbf{e}_V \quad \text{with} \quad \mathbf{e}_V = \cos\theta\mathbf{e}_\rho + \sin\theta\mathbf{e}_b, \tag{7}$$

where $V_\rho = \partial V_0/\partial\rho$, $V_b = -[a(\rho)/b\rho](\partial V_0/\partial\varphi)$, $|\nabla V_0| = \sqrt{V_\rho^2+V_b^2}$, and $\mathbf{e}_V$ is a unit vector with $\tan\theta = V_b/V_\rho$.

*The electron wave function in a helical potential.* To find a solution of Eq. (1) let us use the semiclassical, or WKB, approximation,[11] i.e., look for a solution

$$\Psi(\mathbf{r}) = e^{(i/\hbar)S}\Phi, \tag{8}$$

where $S\equiv S(\mathbf{r})$ is phase function (action) and $\Phi\equiv\Phi(\mathbf{r})$ is spinor function (probability density amplitude). Substitution of (8) into (1) results in the set of equations completely equivalent to Eq. (1):

$$\begin{aligned} &\left[\frac{1}{2m}(\nabla S)^2-(E-V_0)+\frac{\hbar}{4m^2c^2}(\boldsymbol{\sigma}\times\nabla V_0)\cdot\nabla S\right]\Phi \\ &\quad=\frac{\hbar^2}{2m}\Delta\Phi, \\ &(\Delta S)\Phi+2\nabla S\cdot\nabla\Phi+\frac{\hbar}{2mc^2}(\boldsymbol{\sigma}\times\nabla V_0)\cdot\nabla\Phi=0. \end{aligned} \tag{9}$$

In semiclassics the term with $\hbar^2$ in the right-hand part of the first equation is neglected and there it is an equation describing the phase fronts of an electron wave. On the analogy with geometrical optics, an electron ray is a line or curve that is orthogonal to wave fronts $S(\mathbf{r})=\text{const}$ and a $\nabla S$ is proportional to the wave number along this line. For the given potential $V_0(\mathbf{r})$ and the fixed energy $E$ electron trajectories are equipotential helical lines. We ascribe to these lines the direction assuming that the positive direction at each point corresponds to such a direction of $z$. If a radius-vector $\mathbf{r}(l)$ of a point which is placed on the line (2) is considered as a function of arc length $l$ of the ray [natural or arc-length parametrization at which $\tau = l/a(\rho)$ in (2)] then for $S$ at this point one can write down

$$\nabla S = \hbar k\frac{d\mathbf{r}(l)}{dl} = \hbar k\mathbf{e}_t. \tag{10}$$

Taking into account (7) and (10) in the first equation of (9) and neglecting the right-hand part we obtain

$$\left[\frac{\hbar^2k^2}{2m}+V_0-E-\frac{\hbar^2 q_{SO}k}{m}(\mathbf{e}_t\times\mathbf{e}_V)\cdot\boldsymbol{\sigma}\right]\Phi=0, \tag{11}$$

where the wave number

$$q_{\text{SO}} = \frac{|\nabla V_0|}{4mc^2} \tag{12}$$

characterizes in fact a strength of SOI induced by $|\nabla V_0|$. Note, that a SOI, like the last term in the brackets of Eq. (11) and usually referred to as the Rashba SOI,[12] is of intensive research, experimental and theoretical, in quasi-two-dimensional semiconductor structures such as quantum wells and heterostructures.[13] The parameter which characterizes a strength of such SOI, is usually written as $\alpha_{\text{SO}} = \hbar\lambda|\nabla V_0|$. Therefore, this parameter is connected with parameter (12) by the relation

$$\alpha_{\text{SO}} = \frac{\hbar^2 q_{\text{SO}}}{m}. \tag{13}$$

Equation (11) has a solution if $\Phi$ is proportional to the eigenspinor of the matrix $(\mathbf{e}_t\times\mathbf{e}_V)\cdot\boldsymbol{\sigma}$ only. Taking into account (6) and (7) one obtains

$$(\mathbf{e}_t\times\mathbf{e}_V)\cdot\boldsymbol{\sigma} = \begin{pmatrix} -\cos\gamma & e^{-i(\varphi+\phi)}\sin\gamma \\ e^{i(\varphi+\phi)}\sin\gamma & \cos\gamma \end{pmatrix}, \tag{14}$$

where

$$\cos\gamma = \frac{2\pi\rho}{a(\rho)}\cos\theta, \quad \tan\phi = \frac{b}{a(\rho)}\cot\theta. \tag{15}$$

Hence $\Phi = A\chi_\sigma$, where scalar multiplyer $A$ as a function has the same symmetry as the potential $V_0$, and $\chi_\sigma = (u_1 \quad u_2)^T$ is the solution of equation $(\mathbf{e}_t\times\mathbf{e}_V)\cdot\boldsymbol{\sigma}\chi_\sigma = \sigma\chi_\sigma$

with $\sigma$ being the eigenvalue. The matrix (14) has eigenvalues $\sigma = \pm 1$ for two orthonormal spinors

$$\chi_+ = \begin{pmatrix} e^{-i[(\varphi+\phi)/2]} \sin\frac{\gamma}{2} \\ e^{i[(\varphi+\phi)/2]} \cos\frac{\gamma}{2} \end{pmatrix}, \qquad \chi_- = \begin{pmatrix} -e^{-i[(\varphi+\phi)/2]} \cos\frac{\gamma}{2} \\ e^{i[(\varphi+\phi)/2]} \sin\frac{\gamma}{2} \end{pmatrix}. \tag{16}$$

Therefore, the SOI defines the spin quantization axis, and the explicit form of Eq. (11) becomes, depending on the electron spin projection,

$$\frac{\hbar^2 k^2}{2m} - \sigma \frac{\hbar^2 q_{SO} k}{m} + V_0 - E = 0. \tag{17}$$

This equation gives either the energy dependence upon the wave number $k$ along the ray,

$$E_\pm(k) = \frac{\hbar^2 (k \mp q_{SO})^2}{2m} - \frac{\hbar^2 q_{SO}^2}{2m} + V_0\,, \tag{18}$$

or the wave number at the given energy,

$$k_\sigma = \pm\sqrt{\frac{2m}{\hbar^2}(E - V_0) + q_{SO}^2} + \sigma q_{SO} = q + \sigma q_{SO}. \tag{19}$$

In Eq. (19) we have introduced the running wave number

$$q = \pm\sqrt{\frac{2m}{\hbar^2}(E - V_0) + q_{SO}^2}, \tag{20}$$

which determines the velocity of an electron propagation along the helical ray with a given energy. Indeed, for velocity we have $v = (1/\hbar)(dE_\pm/dk) = \hbar(k \mp q_{SO}/m = \hbar q/m)$. Signs "±" in (20) correspond to motion in positive and negative directions, respectively.

Thus, according to the definitions (10) and (19) there are two solutions for phase function $S_\sigma$. Bearing in mind the directional derivative of $S$ along the helical trajectory pointed to by the vector $\mathbf{e}_t$ one can see that $dS/dl = \nabla S \cdot \mathbf{e}_t = \hbar k$. Because $k_\sigma$ are constant along a trajectory, solutions for $S_\sigma$ have the form

$$S_\sigma = \hbar k_\sigma l + F = \hbar(q + \sigma q_{SO}) l + F, \tag{21}$$

where the integration constant $F$ has the same symmetry as the potential and can be included in $A$.

So, the desired functions in the helical potential are

$$\Psi_{q,\sigma} = A_\sigma e^{i(q+\sigma q_{SO})l} \chi_\sigma, \tag{22}$$

where spinors $\chi_\sigma$ are determined in (16). These eigenfunctions describe a curvilinear propagation of electrons along helical rays with definite vectors of the SP: $\mathbf{P}_\sigma = \langle \chi_\sigma | \boldsymbol{\sigma} | \chi_\sigma \rangle$, $\mathbf{P}_- = -\mathbf{P}_+$.

Therefore the SOI acting on the moving electron in the helical potential breaks the spin degeneracy: the spin degenerate one-dimensional (along the electron ray) band $E(k) = \hbar^2 k^2/2m$ splits in the momentum space by $2q_{SO}$ into subbands (18). This is general consequence of a Rashba-like SOI for a quasi-one-dimensional propagation of electrons along curved lines. While Eq. (18) is the result of the nearly free electrons approximation, the same conclusion can be obtained also in the tight-binding approximation.[14]

In general, the eigenstate of an electron, which propagates in some direction with the energy $E$, is described by a superposition of the functions (22). This superposition can be written down as $\Psi_q(l) = A\exp(iql)\chi(l)$ where the spinor $\chi(l) = \sum_\sigma a_\sigma \exp(i\sigma q_{SO} l)\chi_\sigma = [u_\uparrow(l) \quad u_\downarrow(l)]^T$ describes the spin orientation, where $\sum_\sigma |a_\sigma|^2 = 1$. So, if $\chi(l = 0)$ does not coincide with the eigenspinor, the $z$ component of the SP vector $|u_\uparrow(l)|^2 - |u_\downarrow(l)|^2$ is the oscillating function of the variable $l$ with the wave number $2q_{SO}$. These oscillations with necessity lead to the CISS effect. To demonstrate this, the electron transmission through the chiral barrier is considered below.

*The transmission coefficient (TC).* Let the barrier be located between $z = 0$ and $z = d$. It divides the space in three parts: left L ($z < 0$), central C ($0 < z < d$), and right R ($z > d$) ones. In the parts L and R the potential is constant and can be put to zero, meaning that the electron is (quasi)free. In these regions, the phase equals $S = \hbar\mathbf{k} \cdot \mathbf{r}$ with arbitrary coordinate independent spinor. In the part C, the solution of Eq. (1) is given by the expression (22). To obtain the TC, consider a certain situation: an electron normally incident upon the barrier from the left side L. In this case the solution of the Schrödinger Eq. (1) can be written as

$$\begin{aligned} \Psi_L &= A_{\text{inc}} e^{ik_E z} \chi_{\text{inc}} + A_{\text{ref}} e^{-ik_E z} \chi_{\text{ref}}, \quad z < 0, \\ \Psi_C &= \sum_{\nu,\sigma} A_{\sigma,\nu} e^{iS_{\sigma,\nu}/\hbar} \chi_\sigma, \quad 0 < z < d, \\ \Psi_R &= A_{\text{tr}} e^{ik_E z} \chi_{\text{tr}}, \quad z > d. \end{aligned} \tag{23}$$

Here $A_{\text{inc}}$, $A_{\text{ref}}$, and $A_{\text{tr}}$ are amplitudes of incident, reflected, and transmitted electron waves, correspondingly, and the wave number $k_E$ is related to the energy via $k_E = \sqrt{2mE/\hbar^2}$, $S_{\sigma,\nu} = \hbar k_{\sigma,\nu} l$ with $k_{\sigma,\nu} = \nu q + \sigma q_{SO}$ where $\nu = \pm 1$ denotes the direction of the velocity and $q = \sqrt{2m(E - V_0)/\hbar^2}$ [see Eq. (20)].

In the functions (23), the coefficients $A$ and the components of spinors $\chi_{\text{ref}}$ and $\chi_{\text{tr}}$ have to be found from the boundary conditions at $z = 0$, $z = d$. The wave function and its derivatives have to be continuous, so

$$\begin{aligned} \Psi_L(z = 0) &= \Psi_C(l = 0), \quad \nabla\Psi_L(z = 0) = \nabla\Psi_C(l = 0), \\ \Psi_C(l = \mathcal{L}) &= \Psi_R(z = d), \quad \nabla\Psi_C(l = \mathcal{L}) = \nabla\Psi_R(z = d), \end{aligned}$$

where $\mathcal{L} = (a(\rho)/b)d$. These conditions give equations for the coefficients. Let $A_{\text{inc}} = 1$, $\chi_{\text{inc}} = (e^{-i\beta/2}\cos(\delta/2)$ $e^{i\beta/2}\sin(\delta/2))^T$, and $u_\uparrow$ and $u_\downarrow$ are the components of $\chi_{\text{tr}}$. Then one can eliminate the coefficients $A_{\sigma,\nu}$ and $A_{\text{ref}}$ from the equations and solve for unknown components $A_{\text{tr}} u_\uparrow$ and $A_{\text{tr}} u_\downarrow$. In this case $|\Psi_{\text{tr}}|^2 = |A_{\text{tr}}|^2(|u_\uparrow|^2 + |u_\downarrow|^2) = |A_{\text{tr}}|^2 \equiv T$ gives the final TC value,

$$T = \frac{1}{|D|^2} \simeq \frac{4k_E^2 q^2}{4k_E^2 q^2 + \left(k_E^2 - q^2\right)^2 \sin^2 q\mathcal{L}} \tag{24}$$

with $D = \cos q\mathcal{L} - i[(k_E^2 + q^2 - q_{SO}^2/2k_E q)] \sin q\mathcal{L}$ and

$$|u_\uparrow|^2 = \cos^2\frac{\delta}{2} + \Delta u, \quad |u_\downarrow|^2 = \sin^2\frac{\delta}{2} - \Delta u. \tag{25}$$

Therefore, at $q_{SO}^2 \ll k_E^2$ the expression (24) coincides with the well-known formula for a TC of a quantum particle over a potential barrier.[11] The SP factor determined as $P = (T_\uparrow - T_\downarrow)/(T_\uparrow + T_\downarrow) = |u_\uparrow|^2 - |u_\downarrow|^2 = \cos\delta + 2\Delta u$

corresponds to the $z$ component of the polarization vector $\mathbf{P}$ of a transmitting electron which depends on the spin polarization of an incident electron, the strength of the SOI, and the width of a monolayer:

$$\begin{aligned} P = {} & \cos\delta + \sin\delta \sin\gamma \sin(\varphi + \phi - \beta) \sin 2q_{SO}\mathcal{L} \\ & - [\cos\delta \sin^2\gamma + \sin\delta \sin\gamma \cos\gamma \cos(\varphi + \phi - \beta)] \\ & \times \sin^2 q_{SO}\mathcal{L}. \end{aligned} \tag{26}$$

*Conclusion.* Above we calculated TC for the model situation when an electron with arbitrary spin orientation (described by two parameters—polar angles $\delta$ and $\beta$) is normally incident upon the plane-parallel region with the helix-shaped potential. In the experiments,[2,4] photoelectrons emitted from the gold surface are transmitted through the SAM of dsDNA at energies above vacuum level. The dsDNA molecules are rigid and form well-organized monolayers of rigid chiral rods closely packed together.[2,4] Hence, in such monolayers, the potential with well defined helical symmetry can exist for external electrons. Electron transmission is mostly a one-particle process and therefore obtained analytical expressions for transmission of unbounded electrons through the helical potential can describe some features of such processes.

The solution depends on the explicit form of the potential $V_0(\mathbf{r})$. The electrostatic field in the SAM must arise from all electrons and nuclei that comprise the dsDNA molecule and its neighbors. The calculation corresponding potentials is a complicated problem and usually some simplified models are used.[8,9] To make a phenomenological estimation of the polarization effect, let us take into account the DNA structure. The Watson-Crick double helix structure of the DNA molecule has diameter $\approx 20$ Å and contains two grooves—major and minor; the major groove being wider than the minor one. Many proteins which bind to DNA do so through a wide groove. In what follows, we assume that inequality $E - V > 0$ takes place for trajectories which are close to the helical line $\mathbf{r}_0(\tau)$ (2) with $\rho = R_0$ and $\varphi = \varphi_0$, which passes through the major groove. For other rays $E - V < 0$, the quantity $q$ becomes imaginary and the wave function is exponentially decaying within such trajectories. In other words, in order to get insights into the behavior of the SP, we will assume that an electron as a quasifree particle passes through the SAM along the ray near the most probable trajectory $\mathbf{r}_0(\tau)$ in the major grooves of DNA molecules.

Under such assumptions one can use Eq. (26) with $\rho = R_0$ and $\varphi = \varphi_0$ for very rough estimation of the polarization effect considering $q_{\rm SO}$, (12), or $\alpha_{\rm SO}$, (13), as a phenomenological parameter.

Equation (26) is in qualitative agreement with experimental observations—the polarization is energy independent; the selectivity increases with the width (the length of dsDNA) of the monolayer and at $q_{\rm SO}\mathcal{L} \ll 1$ gives linear dependence on dsDNA length $d = \Delta z N$ with $N$ and $\Delta z$ being the number of base pairs in dsDNA and the distance between them along the molecular axis, correspondingly.

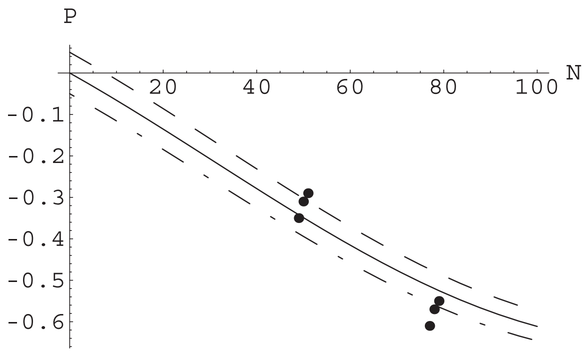

FIG. 1. The longitudinal spin polarization of transmitted electrons, Eq. (26), as function of numbers of base pairs in dsDNA, $N$, for transverse spin polarized, $\delta = \pi/2$ (central solid line) and with small longitudinal component of spin polarization vector, $\delta = \pi/2 \mp 0.2$ (parallel and antiparallel to the direction of propagation), incident electrons. Filled circles indicate experimental points for photoelectrons with linearly polarized (central points) and circularly (clockwise and counterclockwise) polarized light at $N = 50$ and $N = 78$ given in Ref. 4. The effective SO coupling is taken to be $\alpha_{\rm SO} = 1.33$ meV nm which corresponds to $q_{\rm SO}\Delta z = 6 \times 10^{-3}$. Other parameters used are $b = 34$ Å, $\Delta z = 3.4$ Å, $R_0 = 5$ Å and also correspond to DNA molecule.

In Fig. 1 the longitudinal polarization of transmitted electrons (26) as a function of numbers of base pairs in dsDNA is present. In the calculations, $\alpha_{\rm SO} = 1.33$ meV nm is used. This value is close to a physically meaningful estimation of the SOI coupling parameter performed in Ref. 9. The values of $\alpha_{\rm SO} = 1.87$–$2.35$ meV nm are obtained. The situation of highly packed SAMs can be compared to that of semiconductors, in the sense that a molecule such as DNA contains a large number of atoms per turn. Note that for semiconductor heterostructures, values of the parameter $\alpha_{\rm SO}$ (referred to as the Bychkov-Rashba parameter $\alpha_{\rm BR}$) inferred from experimental measurements vary in the range up to 40 meV nm.[13] In this sense, the value $\alpha_{\rm SO} \sim 2$ meV nm corresponds to moderate coupling. In Fig. 1 filled circles indicate experimental points taken from Ref. 4. Thus, obtained results show that such a SOI coupling parameter can provide a rather good qualitative and quantitative agreement with the experimental data.[4]

Of course, the developed theory can be applied to experiments with completely spin-polarized electron beams in which all electrons are in the same spin state. The description of real experiments when electrons of the beam have different spin polarization requires the use of the density matrix formalism, which is beyond the scope of the approach developed in this paper.

*Acknowledgments.* We thank L. S. Bryzhik for technical assistance. This investigation was carried out in the framework of Special Programm of Fundamental Researches of National Academy of Sciences of Ukraine.

---

[*] eremko@bitp.kiev.ua
[†] vloktev@bitp.kiev.ua

[1] K. Ray, S. P. Ananthavel, D. H. Waldeck, and R. Naaman, Science **283**, 814 (1999).

[2] S. G. Ray, S. S. Daube, G. Leitus, Z. Vager, and R. Naaman, Phys. Rev. Lett. **96**, 036101 (2006).

[3] R. Naaman and Z. Vager, MRS Bull. **35**, 429 (2010)

[4] B. Göhler, V. Hamelbeck, T. Z. Markus, M. Kettner, G. F. Hanne, Z. Vager, R. Naaman, and H. Zacharias, Science **331**, 894 (2011).

[5] Z. Xie, T. Z. Markus, S. R. Cohen, Z. Vager, R. Gutierrez, and R. Naaman, Nano Lett. **11**, 4652 (2011).

[6] R. Naaman and D. H. Waldeck, J. Phys. Chem. Lett. **3**, 2178 (2012).

[7] S. S. Skourtis, D. N. Beratan, R. Naaman, A. Nitzan, and D. H. Waldeck, Phys. Rev. Lett. **101**, 238103 (2008).

[8] S. Yeganeh, M. A. Ratner, E. Medina, and V. Mujica, J. Chem. Phys. **131**, 014707 (2009).

[9] R. Gutierrez, E. Díaz, R. Naaman, and G. Cuniberti, Phys. Rev. B **85**, 081404(R) (2012).

[10] A.-M. Guo and Q.-F. Sun, Phys. Rev. Lett. **108**, 218102 (2012).

[11] A. S. Davydov, *Quantum Mechanics* (Pergamon, Oxford, 1976).

[12] E. I. Rashba, Fiz. Tverd. Tela **2**, 1224 (1960) [Sov. Phys. Solid State **2**, 1109 (1960)]; Yu. A. Bychkov and E. I. Rashba, Pisma Zh. Eksp. Teor. Fiz. **39**, 66 (1984) [JETP Lett. **39**, 78 (1984)].

[13] J. Fabian, A. Matos-Abiague, C. Ertler, P. Stano, and I. Žutić, Acta Phys. Slov. **57**, 565 (2010).

[14] The tight-binding approximation is considered in Ref. 9. For the model with the nearest-neighbor hopping approximation, the Hamiltonian can be diagonalized: $H = \sum_{k,\sigma} E_\sigma(k) a^\dagger_{k,\sigma} a_{k,\sigma}$. Here $\sigma = \pm 1$ is the spin and (in the notations of Ref. 9) $E_\pm(k) = U_0 + 2V_{\mathrm{eff}} \cos(k \pm q_{SO})a$ with $a$ being the lattice constant, $V_{\mathrm{eff}} = V\sqrt{1 + (|W|/V)^2}$ and $\tan q_{SO}a = |W|/V$. The parameters $V$ and $W$ describe hopping without and with spin flip due to the SOI.