Electronic states and persistent currents in nanowire quantum ring

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The new model of a quantum ring (QR) defined inside a nanowire (NW) is proposed. The one-particle Hamiltonian for electron in [111]-oriented NW QR is constructed taking into account both Rashba and Dresselhaus spin-orbit coupling (SOC). The energy levels as a function of magnetic field are found using the exact numerical diagonalization. The persistent currents (both charge and spin) are calculated. The specificity of SOC and arising anticrossings in energy spectrum lead to unusual features in persistent current behavior. The variation of magnetic field or carrier concentration by means of gate can lead to pure spin persistent current with the charge current being zero.

I. INTRODUCTION

The recent progress in nanowire (NW) growth technology, in particular, the possibility of radial (core-shell)\textsuperscript{1} and axial\textsuperscript{2} heterostructure growth, leads to the opportunity to fabricate various NW-based structures, e.g. so-called NW-quantum dots (quantum dot inside NW) and other more complex ones. We suppose that the quantum ring (QR) can be grown in NW by similar way (see Fig. 1a), e.g. using well-known hetero-pair GaAs – Al\textsubscript{1-x}Ga\textsubscript{x}As with n-doped Al-rich barriers.

Alternatively, the tubular electron gas (TEG) formed close to InAs-NW surface\textsuperscript{3} can be electrostatically confined to form QR, by analogy with confinement of carriers in carbon nanotubes to ring geometry\textsuperscript{4}. Both mentioned structures significantly differ from known QRs defined in two-dimensional electron gas (2DEG) structures. Especially, the effects that are due to spin-orbit coupling (SOC) will be different.

QRs constitute the polygon for study such coherent effects as Aharonov-Bohm (AB) one\textsuperscript{5} and persistent currents (PCs)\textsuperscript{6}. Usually zero-temperature PC can be found by using the well-known equation

\begin{equation}
I = -c \sum_n \frac{\partial E_n}{\partial \Phi},
\end{equation}

where $E_n$ is the energy levels in the ring, $\Phi$ is the magnetic flux through the ring and the summation is over all occupied states.

The presence of SOC leads to modification of energy spectrum and as a consequence to PC modification. The spectrum of thin (one-dimensional) QR defined in 2DEG structure with Rashba SOC\textsuperscript{7} is well known\textsuperscript{8,9}. However, the lack of inversion center in host semiconductor material leads to other type of spin-splitting\textsuperscript{10} (known as Dresselhaus SOC), that appear in a new light in low-dimensional structures\textsuperscript{11} and particularly in QR-structures\textsuperscript{12}.

Here we will study only features of PCs that are due to specifics of spectrum and SOC, and neglect the disorder and interaction effects. We present the model of thin QR which is confined inside [111]-oriented NW (it is the usual growth direction for NWs of Al\textsubscript{1-x}Ga\textsubscript{x}V materials with zinc-blende lattice). It should be noted, that SOC in NW QR sufficiently differs from SOC in planar QR, where effective Rashba field is constant at each point, and Dresselhaus SOC is different as well due to another crystallographic orientation. It is worth noted, that there is no difference between AB-flux and homogeneous magnetic field for model of thin one-dimensional QR if $g = 0$. However, it seems to be unreal to realize AB-flux through the NWQR, and we discuss here only the case of homogeneous magnetic filed.

II. MODEL AND HAMILTONIAN

Using one-particle Hamiltonian of NW with TEG\textsuperscript{13,14}, that takes into account both Rashba and $k$-linear Dresselhaus SOC, after dimension quantization along NW axis, we find the following effective-mass Hamiltonian for carriers in NWQR

\begin{equation}
H = \frac{\hbar^2}{2m} K^2 \varphi + \alpha \sigma_z K \varphi - \frac{\beta}{2\sqrt{3}} \left( \sigma_z K \varphi - \frac{i}{2r_0} \sigma_\varphi \right) + \sqrt{\frac{3}{2}} \beta \sigma_z \left( \sin 3 \varphi K \varphi - \frac{3i}{2} \cos 3 \varphi \right) + \frac{1}{2} g \mu_B \sigma_z B, \tag{2}
\end{equation}

where the total Hamiltonian consists of kinetic term, Rashba SOC, isotropic and anisotropic Dresselhaus SOC terms, and Zeeman splitting, respectively. Here $K_\varphi = r_0^{-1} (-i \partial / \partial \varphi + \Phi / \Phi_0)$ with $\Phi = \pi r_0^2 B$ being the flux of the magnetic field $B$, and $\Phi_0 = 2\pi \hbar c / |e|$ is the flux quantum, $m, \alpha, \beta, g$ and $r_0$ are the effective mass, Rashba and $k$-linear Dresselhaus SOC parameter, effective g-factor and QR radius, respectively. Here we use the polar Pauli matrices $\sigma_i = \cos \varphi \sigma_x + \sin \varphi \sigma_y$, $\sigma_\varphi = -\sin \varphi \sigma_x + \cos \varphi \sigma_y$, that connected with usual Cartesian Pauli matrices $\sigma_i$ ($i = x, y, z$). The constant energy shift that is due to dimension quantization is omitted in Eq. (2).

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The spectral problem for Hamiltonian (2) can be solved only numerically, but any appropriate set of basis functions can be used for numerical diagonalization. One can see that the Hamiltonian without penultimate term commutes with $z$-projection of total angular momentum, $j_z = -i\hbar \partial / \partial \varphi + (\hbar / 2) \sigma_z$ and therefore it can be diagonalized analytically. Thus, it is convenient to use the eigenfunction of such reduced Hamiltonian for diagonalization of Hamiltonian (2). The result of numerical diagonalization is depicted in Fig. 1, where we restrict ourselves by $40 \times 40$ matrix that ensures the perfect precision for depicted levels. The numerical calculation was performed with material parameters that are typical for InAs-based structures for which SOC-effects are more pronounced. One can see the presence of ‘gap’ (anticrossings) at the spectrum that is due to penultimate term in Hamiltonian (2). It should be noted, that the energy levels will permute at $g = 0$.

Additionally, we can calculate the one-particle density of states (DoS) (see Fig. 1(c)) using the Green’s function of Hamiltonian

$$\text{DoS}(E) = -\frac{1}{\pi} \text{Im} \text{Tr}[(E - H + i\gamma)^{-1}], \quad (3)$$

where $\gamma$ describes the level broadening.

III. PERSISTENT CURRENTS

Since we know the energy spectrum, then we can use Eq. (1) to find PC numerically. However, it is convenient to use the equilibrium density matrix formalism, and to calculate PC by using equation

$$I = \frac{e}{2\pi r_0} \text{Tr}[v_{\varphi} f_0(H, \mu, T)], \quad (4)$$

where $f_0(E, \mu, T)$ is the Fermi distribution function, $E$, $\mu$ and $T$ are the energy, chemical potential and temperature, respectively. This approach is more general and permits to find current at finite temperature. In this case we have to know the matrix elements of velocity operator $v_{\varphi}$ that in turn can be found from Heisenberg equation of motion, $v_{\varphi} = -(i/\hbar)[r_0 \varphi, H]$.

There are possible two different situations: (i) the constant particle number, $N = \text{const}$, that e.g. can be realized in QR defined in core-shell NW-structure and (ii) the constant chemical potential, $\mu = \text{const}$, that can be realized in electrostatically confined TEG in InAs-NW. In the first case one has to additionally find the dependence $\mu(\Phi)$ using well-known relation, $N = \text{Tr}[f_0(H, \mu, T)]$. In the case of $\mu = \text{const}$ the abrupt change in PC occurs near the crossing of energy levels with the chemical potential, whereas in $N = \text{const}$ case it happens close to level crossing (anticrossing).

The numerical calculation of PC as a function of magnetic flux at $\mu = \text{const}$ is depicted in Fig. 2. One can see the usual saw-toothed behavior for the high chemical potential (Fig. 2a) at zero temperature, but there is no $\Phi_0$-periodicity due to non-zero g-factor. The increasing of the temperature leads to smoothing of $I(\Phi)$-dependence. When the chemical potential lies in a ‘gap’ the PC behavior is significantly different. In this case $I(\Phi)$-dependence is smoothly oscillatory even at $T = 0$ (see Fig. 2b).

It is interesting to study persistent spin current (PSC) as well. Usually, the spin current is the pseudo-tensor $I^j_\varphi$ ($i, j = x, y, z$), that components describe the spin component $s_i$ carrying in $j$-th spatial direction. In our case of thin QR there is only one coordinate direction, tangential to QR circumference, i.e. in our case we deal with pseudo-vector $I^j_\varphi \equiv I^j$ ($i = r, \varphi, z$). Here we use the simple definition of spin-current operator and PSC can be found from Eq. (4) with replacement

$$\varepsilon v_{\varphi} \rightarrow \frac{\hbar}{4}(\sigma_i v_{\varphi} + v_{\varphi} \sigma_i). \quad (5)$$

Numerical calculations show that at specific values of magnetic field and chemical potential there is possibility...
to observe a pure PSC, i.e., in this case charge current is zero (see for instance Ref. [15]). The realization of pure PSC is convenient with help of electric gates, that can control not only electron concentration, but the SOC parameter $\alpha$ and in a less degree $\beta$.

IV. CONCLUSION

In conclusion, we proposed two models of QR defined in zinc-blende NWs and constructed the one-particle Hamiltonian for electron in NWQR taking into account both Rashba and $k$-linear Dresselhaus SOC. The specificity of spin-orbit terms in [111]-oriented QR manifests in energy levels and PCs. The energy levels as a function of magnetic field are found revealing several anticrossings that are due to anisotropic part of Dresselhaus SOC. Using the equilibrium density matrix formalism PC and PSC are calculated. Charge and spin PC behavior differs from conventional one, especially for carrier concentration corresponding to the Fermi level position close to anticrossings. The variation of magnetic field or carrier concentration and SOC strength by means of gate can lead to pure spin PC when the charge current is zero.

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