ELECTRONIC STATES IN Bi QUANTUM WIRES UNDER APPLIED LONGITUDINAL UNIFORM MAGNETIC FIELD

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stated as follows: how the longitudinal magnetic field affects the caustics and energy spectrum of the carriers.

To examine carrier states in the nanowire we use the one band approximation. We solve two-dimensional Schrödinger equation to obtain energy spectrum and wave functions of the carrier in the applied magnetic field. The equation was analyzed both numerically and analytically.

I. MATHEMATICAL MODEL

The envelope wave function of the carriers is governed by the effective-mass Schrödinger equation [5],[11]

\[-i\hbar \nabla \phi \Psi(r) = E\Psi(r)\]

\[
H = \frac{hc}{eR}
\]

\[
\frac{H}{\sqrt{M}} = \frac{H}{\sqrt{M}} < \frac{H}{\sqrt{M}}
\]

\[
\frac{\partial \Psi}{\partial \xi} + \frac{\partial \Psi}{\partial \eta} + d(e ch \xi - \eta)\Psi - \frac{i\omega_c \hbar d}{\eta \frac{\partial \Psi}{\partial \xi} - sh \xi \frac{\partial \Psi}{\partial \eta}} = 0
\]

\[
\omega_c = \frac{eH}{c\sqrt{M}}
\]

\[
d = (R/\hbar)\sqrt{(M - M)} R
\]

\[
\Psi_{q p}(\xi, \eta) = \frac{\text{const}}{\sqrt{(\xi) - (\eta)}} \left\{ \frac{id}{\epsilon q p / t_p} \sqrt{(\xi) - (t)dt} \times \right.
\]

\[
\left. \left\{ -i \frac{d}{\epsilon q p / t_p} \left( \frac{\xi}{\eta} \right) \sqrt{(\xi) - (t)dt - i\omega_c \frac{\xi}{\eta}} \right\} \right. 
\]

\[
\left. \left\{ \frac{d}{\epsilon q p / (\xi - \xi) - t_p} \right\} \right. 
\]

\[
\left. v Z \frac{\xi}{\xi} = (\xi) = \sqrt{M/M} \omega_c \right. 
\]

\[
\epsilon q p = \left\{ \frac{\pi}{d} \right\} \left\{ \int_{\sqrt{(\xi) - (\eta)\eta}} \right. \times 
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\[ q + \frac{H}{\eta} + \frac{i_p}{\pi} \left( \frac{H}{\eta} \right)^{\frac{1}{2}} \int_{-\pi}^{\pi} \frac{d\eta}{(\eta - \xi)} \left[ \int_{-\pi}^{\pi} \frac{\xi - (\eta)d\eta}{(\eta - \xi)} \right] \]
Similar effect takes place for the electron with the isotropic transverse mass \[14\]. There are several peculiarities of the carrier space localization obtained in the frame of the anisotropic model. The carrier motion is restricted not only by the elliptic caustics at the nanowire center but also by the arcs of an ellipse and the boundary. Hence, the surface scattering for the carrier of the "whispering gallery" mode is supposed to be small in frame of the anisotropic model. This feature was experimentally observed \[15\].

Fig. 1, 2, 3 show that the probability to find a carrier on the ellipse principal axis between the caustic focuses and the boundary is maximum.

\[
\Psi_{q,p}(\xi, \eta) = \frac{\text{const}}{\sqrt{\xi}} \left( d_{\varepsilon q p} \left( \xi - \left( q \pm \frac{1}{2} \right) \left( \xi \right) \right) \right) \times \\
D_q \left[ \sqrt{d \varepsilon_q p} \left( \eta - \omega_c \sqrt{d \varepsilon_q p} \left( \xi \right) \right) \right]
\]

\[
\varphi_{q,p} = d_{\varepsilon_q p} \left( \xi - \left( q \pm \frac{1}{2} \right) \left( \xi \right) \right)
\]

\[
\varepsilon_{q,p} = \left( d \left( \xi \right) \right) \left[ \mp q + \right] 
\]

Fig. 4 Distribution probability density of an electron in the cross-section of the Bi nanowire. "Jumping ball" mode. Magnetic field \( H = 0, q = 2, p = 6 \)

Fig. 5 Distribution probability density of an electron in the cross-section of the Bi nanowire. "Jumping ball" mode. Magnetic field \( H = 0.5H_0 \)

Fig. 6 Distribution probability density of an electron in the cross-section of the Bi nanowire. "Jumping ball" mode. Magnetic field \( H = -0.5H_0 \)
The electrons of the "jumping ball" mode are restricted by the hyperbolic caustics (see Fig. 4). Fig. 5, 6 show that the applied uniform magnetic field bends the hyperbolic caustics. Hence, the available domain of the electrons is changed by the magnetic field. The carriers actually fill only one half of the nanowire cross-section under the influence of the magnetic field. The magnetic field acts in opposite mode upon electrons and holes. So it is possible to separate the electrons and holes of the "jumping ball" mode by means of the magnetic field. This separation is attractive to enhance good thermoelectric properties of the Bi nanowire. Our calculations show that the magnetic field does not considerably affect the electron energy corresponding to the "jumping ball" modes.

III. NUMERICAL COMPUTATION

The above analysis deals with the highly excited states. We have performed the numerical calculations to examine a steady state and low excited states of the electrons into the nanowire cross-section using the technique described in the paper by Yu-Ming Lin, et.al. [11]. The software is written in Mathcad codes.

Fig. 7 shows that the electrons in the steady state tend to be located in the center of the nanowire cross-section. The electrons of the fourth excited state are located near the cross-section.

Fig. 8 Contour plot of the electron distribution density for the fourth excited state into the cross-section of the nanowire under the applied magnetic field.

Fig. 9 Contour plot of the electron distribution density for the sixth excited state into the cross-section of the nanowire under the applied magnetic field.
They look like the electrons corresponding to the "whispering gallery" mode in the short-wave approximation (compare Fig.2, 8). Fig. 5, 6, 9 shows that the electrons of the sixth excited state seem to be restricted by the hyperbolic caustics like the electrons corresponding to the "jumping ball" mode in the short wave approximation. The "jumping ball" mode disappears if the mass anisotropy is switched off (M = M) (see Fig. 11). In this case only the steady state electrons are centered in the nanowire cross-section. The electrons corresponding to the excited states spread round the surface (see Fig. 10, 11). They correspond to the "whispering gallery" mode.

**SUMMARY**

- There are two groups of carriers with anisotropic mass in the Bi nanowire under the applied uniform magnetic field: (i) ("whispering gallery mode") the carriers restricted by the elliptic caustic at the nanowire center and by the arcs of an ellipse near the boundary, (ii) ("jumping ball" mode) the carriers restricted by the hyperbolic caustic.
- The magnetic field affects the elliptic and hyperbolic caustics.
- The magnetic field increases (decreases) both the space localization and eigenvalue of the carriers of the "whispering gallery" mode.
- There is no considerable influence of the magnetic field on the eigenvalue of the carriers of the "jumping ball" mode. The magnetic field only bends the hyperbolic caustics.
- Electrons and holes of the second class can be separated spatially by means of the magnetic field.
- In general, the carriers are not supposed to interact considerably with the nanowire surface due to their space distribution.
- The "jumping ball" mode disappears if the mass anisotropy is switched off.

**REFERENCES**

5. Bejenari, Symposia Professorum, ULIM, 4-5 mai, 2001, Chisinau, Moldova, Materiale Sesiunii stiintifice, Seria Inginerie, p.3.


