An existence of predominant symmetrical spin configuration (spin polarised phase) and "diluted" density of states (pseudo-gap) in a layer under the Fermi level in a quantum wire is predicted. The condition of cross-over from non-polarised phase to polarised one was derived. The transition occurs for sufficiently low electron density in a wire and is accompanied by an acute decrease of electron density of states near the Fermi level. It may result in a corresponding decrease of conductance. A similar effect may exist in a two-dimensional electron gas.

A lot of papers were issued on the theoretical and experimental investigation of low-dimensional systems: quantum wells, wires and dots, and many remarkable phenomena were revealed. Along with a scientific attractiveness of such structures their especial properties might be applied in future microelectronic and optoelectronic devices. Here we concentrate on one of strong correlation effects in quantum wires (QWRs). These very effects can drastically change the properties of electron system with respect to non-interacting electron gas.

One of the most interesting problems arisen recently was connected with so called "0.7 structure". Firstly this miraculous structure was seen in the experiment with a quantum wire structure in 1996 [1]. There was registered a pronounced additional step of a quantum wire conductance quantisation at the level 0.7 of a conductance quantum $G_0 = 2e^2/h$. A bit later an apparent deviation from a conductance quantum was also observed in the most perfect for today long QWRs [2]. They were fabricated by cleaved overgrowth of GaAs/AlGaAs quantum well heterostructures. Even a decrease down to 50% was revealed for 20µ long wire. Worth mentioning that multiple quantization steps visible in the experiment were subject to equal decrease. Later the fractional conductance quantum steps were seen in the experiments of the Copenhagen group [3-5] and even in metallic nanostructures [6].

Recently a novel observation of the 0.7 structure was made in quantum wires manufactured by split-gate technology [7]. The authors saw again an additional step of quantization at the level 0.7$G_0$. The fact that quite different structures revealed the same effect pointed out to its fundamental origin.

For a while there was no adequate explanation consistent with all available experimental data. Attempts to apply the spin and spinless Luttinger liquid theories seemed the most appropriate to unravel the problem. Indeed, these theories gave the corrections to QWR conductance caused by Coulomb interac-
tion between electrons:

\[ G = G_0 \left(1 + V(0)/\pi v_F\right)^{-1/2} \quad (1) \]

where \( V(0) \) represents the Fourier transform \( V(q) \) of the real space interaction potential between electrons for the transfer momentum \( q \) equal to zero, \( v_F \) is the Fermi velocity. However, these corrections have monotonic dependence on the Fermi energy that contradicts with abrupt transition to common integer steps of conductance quantum with rising a gate voltage observed in the experiment and flat plateaux observed in.

When a disorder was involved this also gave rise to an obvious decrease of the conductance but dependent on the electron density in the wire. The calculations fulfilled for realistic QWR wall roughness also revealed a strong dependence of scattering rate on the Fermi energy and subband number. Thus such a scattering can not be at all a feasible reason of conductance deviation because it do not accord with observed flat plateaus (within 5\%) and conductance steps of equal height.

Moreover, the latest experiments discovered an obvious connection of the "0.7 structure" with spin polarization of electrons in a QWR. There was seen a smooth transition of the "0.7 structure" for zero magnetic field to the "0.5 structure" when a magnetic field was going up. This evidence crucially sustains the hypothesis of spontaneous spin polarization of electrons in a QWR firstly put forward in Ref. prior to the experiment. Here we also argue that the spontaneous spin polarisation owes to exchange interaction between electrons in a QWR.

Unfortunately, few papers were so far issued on the topic. A phenomenological explanation of a spontaneous magnetisation of a quasi-one dimensional conducting channel embedded in a Wigner crystal was presented in Ref. In another Ref. the spontaneous polarisation (magnetisation) was merely postulated but its influence on a conductance was thoroughly discussed.

We start the consideration from a two-electron problem. The exchange energy is assumed to be small compared with kinetic energy. Therefore, we employ the Hartree-Fock (HF) approach to describe exchange interaction.

As for Coulomb interaction, it can be put into account in an audible self-consistent way. However, a realistic Coulomb potential in a QWR should be used. Surely, the electrostatic potential induced by internal electrons in a QWR can even blockade the wire conductance. But we adhere to the experimental conditions when the wire was quite penetrable for electrons and electrostatic potential can not influence on the linear response to infinitesimal bias applied to the wire.

According to the HF approach the two-particle wave function looks like

\[ \Psi(x_1, x_2) = \frac{1}{\sqrt{2}}(\psi_1(x_1)\psi_2(x_2) \pm \psi_1(x_2)\psi_2(x_1)) \quad (2) \]
where $\psi_1, \psi_2$ are one-particle wave functions normalised per one electron in a wire; $x_1, x_2$ are the co-ordinates along the wire. The upper sign corresponds to a singlet state (total spin equals $S=0$) and the lower sign corresponds to a triplet ($S=1$).

The HF equations for $\psi_1$ and $\psi_2$ are as follows

\[
\left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{e^2}{\kappa} \int_0^L \frac{\left| \psi_2(x') \right|^2}{|x-x'|} dx' \right) \psi_1(x) \pm \frac{e^2}{\kappa} \int_0^L \frac{\psi_2^*(x') \psi_1(x')}{|x-x'|} dx' \psi_2(x) = E_1 \psi_1(x) \tag{3}
\]

\[
\left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{e^2}{\kappa} \int_0^L \frac{\left| \psi_1(x') \right|^2}{|x-x'|} dx' \right) \psi_2(x) \pm \frac{e^2}{\kappa} \int_0^L \frac{\psi_1^*(x') \psi_2(x')}{|x-x'|} dx' \psi_1(x) = E_2 \psi_2(x)
\]

Here $\kappa$ is a permittivity, $L$ is a wire length. The integrals with constant sign + correspond to Coulomb interaction. Other integrals describe exchange interaction and their sign is determined by spin configuration.

The Coulomb interaction in the equations (3) is considered as perturbation. The unperturbed electron wave function in a one mode quantum wire is

\[
\psi(k,x) = \frac{1}{\sqrt{L}} e^{i k x} \tag{4}
\]

Suppose that two electrons move across QWR in the same direction (left or right moving fields) with sufficiently small longitudinal momentum discrepancy $\hbar \Delta k$ so that

\[
\hbar \Delta k < \hbar/\lambda \tag{5}
\]

where $\lambda$ is an effective screening length ($\lambda < L$) and $L$ is a wire length. According to equs (3) these electrons possess exchange energy almost as great as Coulomb one

\[
(e^2/\kappa L) \ln(\lambda/d) \tag{6}
\]

here $d$ is a QWR diameter.

In our calculations with equs (3) the Coulomb potential $V(x) = 1/\kappa x$ was cut off for distances $x$ smaller than the wire diameter $d$ and larger than effective screening length $\lambda$.

For greater momentum mismatch than that given by the inequality (5) the exchange integrals involve fast oscillating functions and tend to zero. A sign of exchange energy depends on the spin configuration. If electrons have an antisymmetric spin configuration (total spin equals unity) then their space wave function is symmetric and the sign of exchange energy is positive, i.e. the same as that of Coulomb energy. Otherwise, when a total spin equals zero, the exchange energy is negative and reduces total energy of electron system.
the sake of simplicity in further calculations we suppose the exchange energy to be equal to the Coulomb one \((6)\) when the condition \((5)\) is true. Otherwise, it is supposed to equal zero.

This model of exchange interaction was used to solve many-electron problem. It was found out that due to exchange interaction the ground state \((T = 0)\) corresponding to the minimum of the total energy (including kinetic one) can be that of predominant symmetrical spin configuration for electrons near the Fermi level, i.e. spin polarized. The condition of the cross-over from conventional unpolarized state to polarized one is as follows

\[
\lambda_F \ln(\lambda/d) > a_B
\]

where \(\lambda_F = 4a\) is the Fermi electron wave length, \(a^{-1}\) is an electron density in a wire and \(a_B = \hbar^2 \kappa / m e^2\) is a Bohr radius.

To some extent, the above relation reminds the condition of Wigner crystallisation in a quantum wire deduced in Ref. [15]. However, the condition \((7)\) is valid for greater electron density in a QWR if only \(\lambda > a\). In other words, the spin polarisation precedes the Wigner crystallisation.

Once the condition \((7)\) is met the polarized phase arises in the energy interval under the Fermi level

\[
\delta \epsilon = (e^2 / \kappa \lambda) \ln(\lambda/d)
\]

The magnitude of \(\delta \epsilon\) equals the exchange energy per one Fermi electron. Worth mentioning that it does not depend upon Fermi energy of electrons in any subband of a QWR. This is in a good qualitative agreement with the experimental evidence for conductance corrections to be insensitive to the Fermi energy [2]. The spin configuration associated with the polarised state is sketched in Fig.

In polarised state the exchange energy \(\varepsilon_{ex}(k)\) for electrons adjacent to the Fermi level linearly depends upon momentum

\[
\varepsilon_{ex}(k) = 4(e^2 / \kappa)(k - k_F + \Delta k) \ln(\lambda/d)
\]

where \(k_F = 2\pi / \lambda_F\) is the Fermi wave vector. The total energy equals \(\varepsilon = \varepsilon_{ex}(k) + h^2 k^2 / 2m\) (the kinetic energy is added here).

The relation \((9)\) originates from a dependence of an electron exchange energy upon spin configuration of near-by electrons in k-space (Fig.1). Here we put attention to the important point of our consideration. Although the resulting correction to the energy (consequently corrections to the Fermi velocity \(v_F\)) given by exp.(9) may be quite small, a derivative \(d\varepsilon_{ex}/dk\) connected with density of states \(\rho(\varepsilon) \sim (d\varepsilon/dk)^{-1}\) may be large.

From exp. (9) we deduce the relative decrease of electron density of states in the energy interval \(\delta \epsilon\) under the Fermi level as

\[
\Delta \rho / \rho \sim (\pi a_B k_F)^{-1} \ln(\lambda/d).
\]
According to inequality (7) the relative decrease of density of states (10) cannot be less than 0.25 in a spin polarised phase. However, as the parameter in the right hand side of the exp.(10) is not small a non-perturbation approach should be developed to get a precise number.

The spontaneous magnetisation can affect various phenomena in which electrons at the Fermi level are involved. In particular, the "diluted" density of states (or pseudo-gap) may result in corresponding decrease of conductance. Although the main goal of the present paper is to make clear the origin of a spontaneous magnetisation we briefly discuss its influence upon a conductance. The ballistic current through the wire biased by a voltage $V$ can be calculated in the conventional way \[ I = e \int_{\epsilon_F - eV/2}^{\epsilon_F + eV/2} v(\epsilon)\rho(\epsilon)d(\epsilon) \approx e^2v_F\rho(\epsilon_F)V \quad (11) \]

Thus we obtain the same relative correction to the conductance as that given by formula (10) for density of states. Much more elaborate calculation of the conductance was given in Ref. [13]. However, the magnetisation was postulated there. It should be outlined that our approach gives no corrections of the kind supplied by the exp. (1) to a wire conductance in depolarised state. It concords at the best with numerous experiments where integer plateaux of conductance were observed in controversy to the Luttinger liquid theory predictions.

Our estimations show that the condition of crossover (7) to polarised phase was valid even for the top Fermi energies attained in the experiment [2] (unlike to that in [7]). We accepted for evaluations a screening length $\lambda$ as a distance from the QWR to the nearest gate electrode and the wire diameter $d$ consistent with subband spacing (20 meV) pointed out in [2]. Then we gained $\delta\epsilon_F$ exceeding $kT$ (for $T$ about 1K). When the temperature $T$ was rising the polarised phase was smeared and the conductance quantum restated. This explains the abnormal temperature dependence of the QWR conductance seen in the experiment. When the bias $V$ exceeds $\delta\epsilon/e$ "undiluted" electrons were involved in the conductance and a conductance quantum restates too.

To be consistent with over-all experimental data a wire length should be introduced in the theory. The experiment [2] revealed a quite weak dependence of the conductance deviation on the wire length, at least, sub-linear one. The conductance deviation was only doubled while the wire length varied from 1$\mu$m to 20$\mu$m. To possibilities look like plausible. The first one is that in the experimental structure the wire diameter diminishes as the wire lengthens. An indirect insinuation to this very dependence was that less negative gate voltage pinched off a longer wire. The second possibility is an interaction of a wire with leads which partially destroy the polarised phase in the pre-contact region. Although the leads were already modelled in [18-19] this consideration looks quite deficient yet and further attempts are required. Otherwise, the presence of leads would
be an eternal artifice to fit the theory to the experiment.

It should be noted that a similar phenomenon seems quite possible to exist in a two-dimensional electron gas.

In conclusion, an existence of predominant symmetrical spin configuration (spin polarized phase) and "diluted" density of states under the Fermi level in the quantum wire is predicted. The reduction of quantum wire conductance is in agreement with recent experimental data. The condition of cross-over from non-polarised phase to polarised one was derived. The transition occurs for sufficiently low electron density in a wire and is accompanied by an acute decrease of electron density of states near the Fermi level (pseudo-gap) resulting in a corresponding decrease of conductance. The effect crucially depends upon screening.

Acknowledgments
The work was supported through the program "Physics of solid state nanostructures" (grant N 97-1077) and program "Prospective technologies and devices of micro- and nanoelectronics" (grant N 02.04.4.1.32.E.35) of the Russian Ministry of Science, and also through the Russian Basic Research Foundation (grant N 000100397).

References
[1] Thomas K.J. et al. Phys.Rev.Lett. 1996, Vol. 77, P. 135; Phys.Rev.B 1998, Vol. B58, P.4846.
[2] Yacoby A., Stormer H.L., Wingreen N.S., Pfeifer L.N., Baldwin K.W., West K.W. Phys.Rev.Lett. 1996, Vol. 77, P. 4612.
[3] A.Kristiansen et al., J. Appl. Phys.1998 Vol.83,P.607.
[4] A.Kristiansen et al., Physica B 1998,Vol.249-251,P.180.
[5] A.Kristiansen et al., cond-mat/9808007.
[6] C.Shu, C.Z.Li, H.X.He, A.Bogozi, J.S.Bunch, and N.J.Tao. Phys. Rev. Lett.2000,vol.84,P.5196.
[7] Liang C.-T., Simmons M.Y., Smith C.G., Kim G.H., Ritchi D.A., and Pepper M. cond-mat/9907379.
[8] Apel W. and Rice T.M. Phys.Rev. B 1982,Vol.26,P.7063-7065.
[9] Maslov D.L.Phys.Rev.B 1995, Vol.B52,P.R14368.
[10] Fedirko V.A., V’yurkov V.V. Russian Microelectronics 1997, Vol.26,P.216.
[11] Vyurkov V., Fedirko V., and Fedichkin L. Phys. Low-Dim. Struct. 1999, N 3/4, P. 200-226.

[12] B. Spivak, Fei Zhou, cond-mat/9911175.

[13] Bruus H., Cheanov V.V., Flensberg K., cond-mat/0002338.

[14] Sablikov V.A., Shchamkhalova B.S. Phys. Rev. B 1998, Vol. B58, P. 13847.

[15] Vyurkov V. and Fedichkin L. Phys. Low-Dim. Struct. 1995, Vol. 12, P. 277.

[16] Maslov D.L. and Stone M. Phys. Rev. B. 1995, Vol. B52, P. R5539-R5542.

[17] Beenakker C.W.J. and van Houten H., in Solid State Physics, edited by H. Ehrenreich and D. Turnbull (Academic Press, NY, 1991).

[18] Ponomarenko V.V. Phys. Rev. B 1995, Vol. B52, P. R8666-R8667.

[19] Safi I. and Schulz H.J. Phys. Rev. B 1995, Vol. B52, P. R17040-R17043.
FIGURE CAPTION.
Electrons with different orientation of spin (up and down) fill the longitudinal momentum $k$-space states near the Fermi level. The latter coincides with upper electron state in both stacks. Empty squares correspond to unoccupied states. The same situation exists for electrons moving in the opposite direction ($k < 0$).