Conductance structure in a one-dimensional quantum contact: dependence on the longitudinal magnetic field

O.P. Sushkov
School of Physics, University of New South Wales, Sydney 2052, Australia

Very short quantum wires (quantum contacts) exhibit a conductance structure at the value of conductance close to $0.7 \times 2e^2/h$. The structure was discovered by Thomas et al (Phys. Rev. Lett. 77, 135 (1996)). Dependence of the structure on the longitudinal magnetic field was studied in the same experiment. This dependence has clearly demonstrated that the effect is related to the electron spin. In the recent work (Sushkov, Phys. Rev. B 64, (2001)) it was suggested that the effect is caused by the development of the charge density wave within the contact. The many-body Hartree-Fock calculation has confirmed the picture. The exchange electron-electron interaction is crucial for this calculation, so in agreement with experiment the effect is intrinsically related to the spin. However the dependence on the magnetic field has not been calculated yet. In the present paper the many-body Hartree-Fock calculation of conductance in the presence of the longitudinal magnetic field is performed.

PACS: 73.61.-r, 73.23.Ad, 71.45.Lr

The quantized conductance $G = nG_2$, $n = 1, 2, 3, \ldots$, $G_2 = 2e^2/h$, through a narrow quantum point contact was discovered in 1988. This quantization can be understood within a one-dimensional (1D) non-interacting electron gas picture, see e.g. Ref. 1. In the present work we are interested in a deviation from the integer quantization. This deviation, the so-called “0.7 structure” has been found in experimental works. The structure is a shoulder-like feature or a narrow plateau at $G \approx 0.7G_2$. More recent work demonstrates that there are some above barrier excitations related to the structure and that the structure evolves down to $G \approx 0.5G_2$ in longer quantum contacts.

Dependence of the structure on the longitudinal magnetic field was studied already in the pioneering work. This study clearly demonstrated that the effect is somehow related to the electron spin. There have been numerous attempts to explain the “0.7 structure” by spontaneous magnetization of the 1D quantum wire or, or by the formation of a two-electron bound state with nonzero total spin. However these scenarios contradict to the rigorous Lieb-Mattis theorem that claims that a 1D many-body system with a potential interaction has zero spin in the ground state.

In the recent work I have suggested that the effect is caused by the development of the charge density wave within the contact. This wave is a precursor for 1D Wigner crystallization. The total spin of the system without a magnetic field is zero in agreement with the Lieb-Mattis theorem. The many-body Hartree-Fock calculation has confirmed the picture and reproduced the “0.7 structure”. The exchange electron-electron interaction is crucial for this calculation, in this sense the effect is intrinsically related to spin. However to probe explicitly the spin dependence one has to follow the path of the experiment and to calculate the quantum contact conductance in the presence of the longitudinal magnetic field. Such calculation is performed in the present work.

The present work employs the same technique that has been developed in Ref. 4. This is the Hartree-Fock (HF) method combined with the fictitious gauge field method. However there are some complications that are due to the magnetic field. Let us first formulate the idea of the approach. In independent particle approximation, i.e. in the case of an ideal electron gas, a calculation of the conductance for a given transverse channel is straightforward

$$G = \frac{2e^2}{h} T,$$  

(1)

where $T$ is the barrier transmission probability at Fermi energy. In case of interacting particles this formula is also valid because before and after the potential barrier the density of electrons is high enough, and hence the interaction is negligible. However one cannot use the single particle description to calculate the transmission probability $T$ because in the vicinity of the barrier the electron density is low, and hence the many-body effects are very important. To calculate the transmission probability $T$ the following method is applied. Consider the liquid of electrons on a 1D ring with a potential barrier somewhere on the ring. There is no current in the ground state of the system. Now let us apply a magnetic flux through the ring. This flux induces the electric current. Note that this is not a real magnetic field, this is a fictitious gauge field that generates the current without applying any voltage. On the one hand the current is related to the barrier transmission probability $T$. On the other hand, the current can be calculated using the HF method. This allows to find $T$ with account of many-body effects.

Now we have to repeat the same calculation with addition of the real longitudinal magnetic field $B$. This field does not influence an orbital dynamics, but it splits Fermi levels for electrons with spin up and spin down. So we
have to perform the HF calculation in the sector with nonzero total spin. According to the experimental data\cite{4,5}, the dependence of the conductance on the gate voltage evolves with the magnetic field. The field influences the 0.7 structure, and at the value of the field $B \approx 5 - 10$ T the conductance evolves to the double step function that one should expect for a simple spin split band. The effective value of the electron $g$ factor depends on the width of the channel. For a wide channel it is close to the bulk limit $g \approx 0.4$, and for a narrow channel it is $g \approx 1$, see Refs.\cite{4,5}. There is only one channel in the quantum contact we are interested in, so the contact is narrow. On the other side the electrons incident on the contact are coming from the bulk and the degree of their polarization is determined by the bulk. Therefore for the estimate we take the intermediate value $g \sim 0.7$. Then the energy splitting corresponding to $B = 5$ T is

$$\Delta E = g \mu_B B = 2 \times 10^{-4} eV = 2 \times 10^{-2} E_{unit}. \quad (2)$$

We use atomic units, so distances are measured in units of Bohr radius, $a_B = \frac{\hbar^2}{me^2}$, and energies are measured in units of $E_{unit} = m \frac{\hbar^2}{e^2}$, where $m$ is the effective electron mass and $\epsilon$ is the dielectric constant. For experimental conditions of works\cite{4–7} these values are the following: $a_B \approx 10^{-2} \mu m$, $E_{unit} \approx 10^{-2} eV$. The energy scale (2) corresponds to the temperature $T \approx 2$ K. It is interesting to note that the "0.7 structure" depends on the temperature exactly on this scale\cite{4–7}. At this stage this is just an observation. In the present work we consider only the case of zero temperature.

The Hamiltonian of the many body system that we consider is of the form

$$H = \sum_i \left[ \frac{(p_i - A)^2}{2} + U(x_i) - 2 g \mu_B B \cdot s_i \right] + \frac{1}{2} \sum_{i,j} V(x_i, x_j), \quad (3)$$

where indexes $i$ and $j$ numerates electrons, $s_i$ is the electron spin, $x_i$ is the periodic coordinate on the ring of length $L$ ($0 < x < L$), $A = \pi/2L$ is the fictitious gauge field, and $B$ is the longitudinal magnetic field. The electron-electron Coulomb repulsion is of the form

$$V(x, y) = \frac{1}{\sqrt{a_t^2 + D(x, y)^2}}, \quad (4)$$

where $a_t \approx 2$ is the effective width of the transverse channel, and $D(x, y)$ is the length of the shortest arc between the points $x$ and $y$ on the ring, for more details see Ref.\cite{17}. To model the gate potential\cite{4–7} we use the following formula for the potential barrier

$$U(x) = \frac{U_0}{e^{(|x| - l/2)/d}} + 1. \quad (5)$$

In the present work we take $l = 10$ and $d = 1$. The plot of $U(x)$ is shown in Fig.1 by a solid line

![Fig. 1. The solid line shows the external potential \(U\) at \(U_0 = 4\). The dashed line shows the compensating potential \(U_c(x)\).](image-url)
It was demonstrated in Ref. 17 that to find the barrier transmission probability at Fermi energy with account of many-body effects one has to solve the many-body problem twice: without the barrier and with the barrier. The ratio of electric currents squared gives the transmission probability $T = \left( \frac{J_U}{J_0} \right)^2$. This formula is valid without an external magnetic field. Repeating considerations of Ref. 17 one can prove that with the magnetic field, i.e. with the spin splitting, the probability is given by

$$T = \frac{1}{2} \left( \frac{J_{U\uparrow}}{J_{0\uparrow}} \right)^2 + \frac{1}{2} \left( \frac{J_{U\downarrow}}{J_{0\downarrow}} \right)^2,$$

where $J_{U\uparrow}$ is the electric current of electrons with spin up and spin down correspondingly. This formula gives the probability and hence due to eq. (1) it solves the many-body problem of conductance.

To solve the many-body problem (3) we use the Hartree-Fock (HF) approximation. In the HF approximation the many body wave function is represented in the form of the Slater determinant of single particle orbitals $\varphi_{i\sigma}(x)$. The index $i$ shows the coordinate state of the orbital, and the index $\sigma = \pm 1/2$ shows the spin state of the orbital. Each orbital obeys the equation

$$\hat{h}\varphi_{i\sigma} = \epsilon_{i\sigma}\varphi_{i\sigma},$$

where $\epsilon_{i\sigma}$ is the single particle energy and $\hat{h}$ is the HF Hamiltonian

$$\hat{h}\varphi_{i\sigma}(x) = \left( \frac{(p-A)^2}{2} + U_{\text{eff}}(x) - g\mu_B B\sigma \right) \varphi_{i\sigma}(x) - \sum_j |\varphi_{j\sigma}^*(y)\varphi_{i\sigma}(y)V(x,y)dy|\varphi_{j\sigma}(x),$$

$$U_{\text{eff}} = U(x) + \sum_{j\sigma} \int |\varphi_{j\sigma}(y)|^2 V(x,y)dy + U_c(x).$$

The summations are performed over all filled orbitals. The compensating potential at this stage is zero, $U_c = 0$. We will use the compensating potential later to deal with some computational problems.

For computations we use a finite grid. In the grid modification of the Hamiltonian (8) the kinetic energy $(p-A)^2$ is replaced by $[2|\varphi(n)|^2 - \varphi(n+1)e^{iAh}\varphi(n) - \varphi(n)e^{-iAh}\varphi(n+1)]/2h^2$. Here $h$ is the step of the grid and $\varphi(n)$ is the wave function on the site $n$ of the grid. The electric current corresponding to the grid Hamiltonian is

$$J_{i\sigma} = -\sum_j \frac{i}{2h} \left( \varphi_{j\sigma}(n)e^{iAh}\varphi_{j\sigma}(n+1) - \varphi_{j\sigma}^*(n+1)e^{-iAh}\varphi_{j\sigma}(n) \right).$$

The current is conserved because of the gauge invariance of HF equations.

In the computations we use the grid of 400 points and the total number of electrons $N = N_{\uparrow} + N_{\downarrow} = 158$. Because of the computational time limitation it is very hard to increase substantially these numbers. The transmission probability versus the external potential $U_0$, see eq. (5), is shown in Fig.2. It has been calculated at zero magnetic field, i.e. at $N_{\uparrow} = N_{\downarrow} = 79$, for the ring of length $L = 80$.

![Fig. 2. The transmission probability versus the external potential barrier height $U_0$. Length of the ring is $L = 80$.](image-url)
The Fig.2 clearly indicates the “0.7 structure”. It was discussed in detail in Ref.17 that the structure is due to the Coulomb exchange interaction on the barrier.

To find the effect of the longitudinal magnetic field one has to repeat the above calculation with the magnetic field. In general terms it is straightforward, but there is a serious technical complication. In the above calculation the density of electrons outside the barrier is $n \approx 158/80 \approx 2$. The corresponding Fermi momentum is $p_F = \sqrt{2\pi n} \approx 3.5$. The electron spectrum is discreet with energy splitting $\delta \epsilon = p_F \pi/L \approx 0.1$. This is ten times larger than the splitting due to the magnetic field 5T. Thus the system is not sensitive to the magnetic field up to $B \sim 50T$. Certainly it is not a physical effect, it is a byproduct of the finite ring method used in the calculation. To resolve the problem in a straightforward way one has to increase the length of the ring by at least an order of magnitude. The density of electrons must be substantially higher than the critical density. It means that the total number of electrons must be at least 1000-2000. This is computationally impossible.

To resolve the problem we use the following combination of the means: 1) Increase the length up to $L = 260$. 2) Make the electron-electron interaction (4) dependent on the position on the ring:

$$V(x, y) \rightarrow V_d(x, y) = \frac{V(x, y)}{\left(e^{(|x| - 15)/2} + 1\right)\left(e^{(|y| - 15)/2} + 1\right)},$$

(10)

3) Introduce into eq. (8) an additional compensating potential $U_c(x)$. The interaction $V_d$ coincides with the Coulomb interaction $V(x, y)$ in the interval [-15, 15], and $V_d$ vanishes outside of this interval. Since there is no interaction at large distances we can have a relatively low density of electrons at $|x| > 15$. There is a prize for the translationally noninvariant interaction $V_d$. Unfortunately the interaction produces the unphysical Coulomb barrier. To compensate the unphysical barrier we introduce the compensating potential $U_c(x)$ adjusted in such a way that in absence of the real potential barrier ($U_0 = 0$, see eq. (3)) the density of electrons at the contact, $-15 < x < 15$, is $n \approx 1$. The compensating potential $U_c(x)$ is shown in Fig.1 by the dashed line. The density of electrons $n(x)$ obtained by solution of HF eqs. with $V_d$ and $U_c$ but without any external barrier ($U_0 = 0$) is shown in Fig.3.

![FIG. 3. Selfconsistent density of electrons calculated with the modified Coulomb interaction $V_d$ and with the compensating potential $U_c$. The external potential is zero, $U(x) = 0$. The length of the ring is $L = 260$.](image)

The energy splitting between single particle levels in this case is $\delta \epsilon \approx 0.01$. The spin flip of a single electron creates an additional spin up electron and an additional spin down hole, so it “costs” $2\epsilon \approx 0.02$. This must be smaller than the magnetic splitting. So the minimal magnetic field we can consider is 5T.

Hartree-Fock calculations for the long ring ($L=260$) with the modified Coulomb interaction (10) and with the corresponding compensating potential $U_c$ are absolutely similar to that described before. In this case the effective potential $U_{eff}$, see eq. (6), is not constant even without any external barrier (3). However this effective potential is smooth and well below the Fermi energy. Therefore it does not influence the transmission probability. So in equation (6) for the transmission probability the current $J_0$ corresponds to the zero external potential, and the current $J_U$ corresponds to some given value of the external potential $U_0$. The transmission probability at zero magnetic field (i.e. $N_\uparrow = N_\downarrow = 79$) versus the barrier height $U_0$ is plotted in Fig.4 by the solid line.
FIG. 4. The transmission probability versus the external potential barrier height $U_0$. This is the Hartree-Fock calculation on the ring of length $L = 260$ with the modified Coulomb interaction. The solid line corresponds to zero magnetic field. The long-dashed line corresponds to the field $B = 5T$, and the dashed line corresponds to $B = 10T$.

One can see that after smearing the average position of the structure is close to $T \approx 0.7$. However compared to Fig.2 the structure is much more pronounced. This happens because the modified Coulomb interaction (10) underestimates the Hartree screening, at the same time the exchange interaction responsible for the structure is not influenced by the modification. Underestimation of the Hartree screening leads also to the shift in the position of the step: it is at $U_0 \sim 3.5$ in Fig.4 and at $U_0 \sim 10.5$ in Fig.2 (full screening). However all these details are not that important, the “0.7 structure” qualitatively and to large extent quantitatively is described. What is important is that the modification gives us the possibility to work with the magnetic field. The result of calculation for $N_\uparrow = 80$ and $N_\downarrow = 78$ is shown in Fig. 4 by the long dashed line. As it was discussed before it corresponds to the field $B = 5T$. The result for $N_\uparrow = 81$ and $N_\downarrow = 77$ is shown by the dashed line. It corresponds to the field $B = 10T$. In agreement with the data the field $B \sim 5T$ shifts the position of the structure close to $T \approx 0.5$. Further increasing of the field practically does not influence the picture.

It is very illustrative to perform also calculations in the Hartree approximation, i.e. calculations without exchange interaction. The results for $B = 0$ (solid line), $B = 5T$ (long-dashed line), $B = 10T$ (dashed line) are plotted in Fig. 5.

FIG. 5. The transmission probability versus the external potential height $U_0$ calculated in the Hartree approximation. The solid line corresponds to zero magnetic field. The long-dashed line corresponds to the field $B = 5T$, and the dashed line corresponds to $B = 10T$. 

5
As one should expect neither “0.7 structure” no magnetic field dependence appear in the Hartree calculation. In conclusion we have performed the many-body Hartree-Fock calculation of conductance in the presence of the longitudinal magnetic field. Results of the calculation are shown in Fig.4 where the transmission probability (the conductance in units $2e^2/h$) is plotted versus the potential barrier height that models the gate potential. The solid line corresponds to zero magnetic field, the long-dashed line corresponds to the field $B = 5T$, and the dashed line corresponds to $B = 10T$. There are some computational limitations related to work with the magnetic field. To overcome these limitations we had to modify the electron-electron Coulomb interaction at large distances. This is why the structure in conductance in Fig.4 is more pronounced than the structure in the calculation without the modification shown in Fig.2. Our calculation demonstrates that the magnetic field $B \sim 5T$ shifts the position of the structure close to $T \approx 0.5$. Further increasing of the field practically does not influence the picture. These results are in qualitative and to a large extent quantitative agreement with the experimental data. The agreement gives further confirmation of the explanation of the “0.7 structure” suggested in Ref.\[17].

1. D. A. Wharam, T. J. Thornton, R. Newbury, M. Pepper, H. Ritchie, G. A. C. Jones, J. Phys. C 21, L209 (1988).
2. B. J. van Wees, H. van Houten, C. W. J. Beenakker, J. G. Williamson, L. P. Kouwenhoven, D. van der Marel, C. T. Foxton, Phys. Rev. Lett. 60, 848 (1988).
3. M. Büttiker, Phys. Rev. B 41, 7906 (1990).
4. K. J. Thomas, J. T. Nicholls, M. Y. Simmons, M. Pepper, D. R. Mace, and D. A. Ritchie, Phys. Rev. Lett. 77, 135 (1996).
5. K. J. Thomas, J. T. Nicholls, N. J. Appleyard, M. Y. Simmons, M. Pepper, D. R. Mace, W. R. Tribe, and and D. A. Ritchie, Phys. Rev. B 58, 4846 (1998).
6. A. Kristensen, H. Bruus, A. E. Hansen, J. B. Jensen, P. E. Lindelof, C. J. Mareckmann, J. Nygård, C. B. Sørensen, F. Beuscher, A. Forchel, and M. Michel, Phys. Rev. B 62, 10950 (2000).
7. D. J. Reilly, G. R. Facer, A. S. Dzurak, B. E. Kane, R. G. Clark, P. J. Stiles, A. R. Hamilton, J. L. O’Brien, N. E. Lumpkin, L. N. Pfeiffer, and K. W. West, Phys. Rev. B 63, 121311 (2001).
8. Chuan-Kui Wang and K.-F. Berggren, Phys. Rev. B 54, 14257 (1996); Phys. Rev. B 57, 4552 (1998).
9. L. Calmels and A. Gold, Solid State Commun. 106, 139 (1998).
10. N. Zabala, M. J. Puska, and R. M. Nieminen, Phys. Rev. Lett. 80, 3336 (1998).
11. V. Vyurkov and A. Vetrov, cond-mat/0008073.
12. B. Spivak and F. Zhou, Phys. Rev. B 61, 16730 (2000).
13. A. M. Bychkov, I. I. Yakimenko, and K.-F. Berggren, Nanotechnology 11, 318 (2000).
14. V. V. Flambaum and M. Yu. Kuchiev, Phys. Rev. B 61, R7869 (2000).
15. T. Rejec, A. Ramšak, and J. H. Jefferson, Phys. Rev. B 62, 12985 (2000).
16. E. Lieb and D. Mattis, Phys. Rev. B 125, 164 (1962).
17. O. P. Sushkov, Phys. Rev. B 64, 15 October (2001), cond-mat/0104006.
18. L. I. Glazman, I. M. Ruzin, and B. I. Shklovskii, Phys. Rev. B 45, 8454 (1992).
19. R. Landauer, Z. Phys. 68, 217 (1987).