

Results of the DFT calculation with the potential detected in the 2DEG plane

In the DFT calculation we unfortunately cannot simulate a device in which both the measured QPC and the detector QPC are present. In order to perform such a calculation we would have to put both QPCs inside a very wide quantum wire. The number of modes such a wire would have to support would be too large for the calculation to be feasible. In the single QPC geometry we used in our DFT calculation we could have measured the potential in the 2DEG plane next to the QPC instead of 200 nm below the 2DEG plane as we did. It turns out that the features observed in the experiment and in our DFT calculation can also be observed if we simulate measuring the potential in the 2DEG plane (see Figure S1.) In Figure S2, the derivative D was calculated from the potential measured in the 2DEG plane 300 nm from the center of the QPC. As in the calculation presented in the paper, there is a large dip at pinch-off and a series of weaker dips corresponding to higher transverse modes being occupied in the QPC. Observation of these features in two different geometries supports our contention that they are qualitatively linked to the features we observe in the experiment. However, because the experimental geometry is different from that of the two calculations we cannot claim that the calculations should quantitatively account for the magnitudes of the dips in the real device.

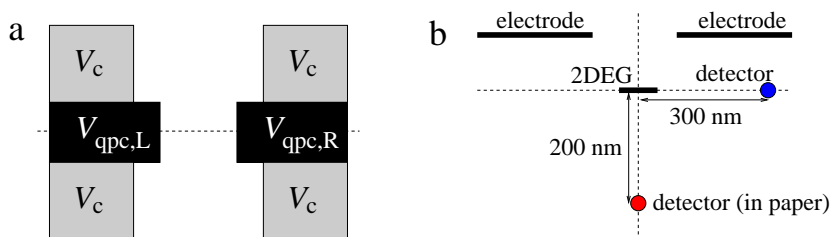


Figure S1: a) The electrodes of the modified QPC used in the DFT calculation. b) The cross section through the center of the QPC (dashed line in panel a). The red dot 200 nm below the 2DEG is the position of the detector in the calculation presented in the paper. The derivative D^{DFT} calculated from the potential in the 2DEG plane 300 nm from the center of the QPC (blue dot) is shown in the next figure. In the calculation presented in the paper the voltages on both gate electrodes were changed together ($V_{\text{qpc,L}} = V_{\text{qpc,R}}$), while in the present calculation $V_{\text{qpc,R}}$ was fixed and we only varied $V_{\text{qpc,L}}$.

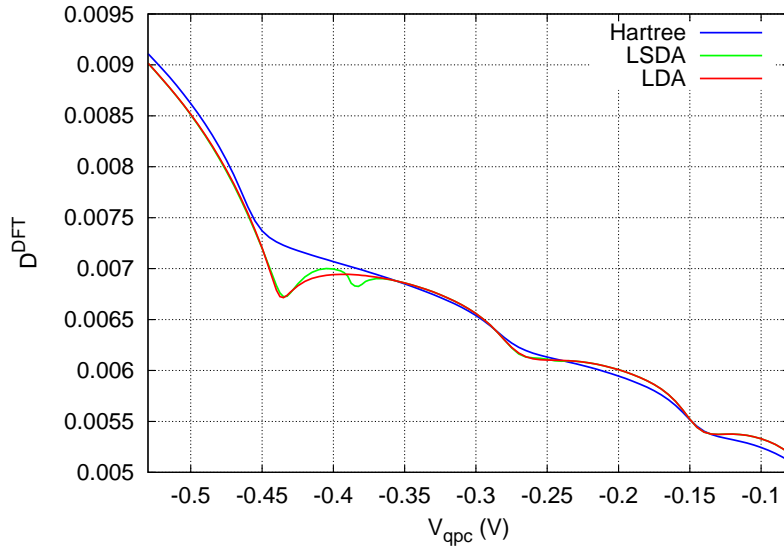


Figure S2: The derivative D^{DFT} calculated from the potential off to the side in the 2DEG plane (detector location is shown as a blue dot in Fig. S1b). The curves for three different approximations are shown: DFT within local density approximation (red), DFT within local spin-density approximation (green) and the Hartree approximation (blue). The curves show very similar behavior to that of the calculation presented in the paper (Fig. 2c and Fig. 3), showing that the detailed geometry is not important in determining the qualitative features of the compressibility measurement, as long as the system under study lies between the gate that is varied and the detector. The magnitude of D^{DFT} , however, is smaller here because the right gate electrode effectively screens the potential. In the experiment, the electrode separating the two QPCs is very thin and is thus less effective in screening the potential.

Adjustable parameters

We did not adjust parameters to try to achieve the best possible fit to the data. Rather, we chose values for parameters as close as possible to the values in the real device while maintaining computational feasibility.

Values for most of the important parameters for the DFT calculation are given in the manuscript. Other relevant parameters are the lithographic width of the quantum wire away from the QPC (300 nm), the voltage on the quantum wire electrodes ($V_c = -0.08V$) and the position of the donor layer (20 nm below the surface). The details of our numerical approach are presented in a separate publication [1].

Can spin rearrangement be detected with our method?

The additional dip near pinch-off in the local spin-density approximation (LSDA) calculation is related to formation of a spin-1/2 magnetic moment in the QPC. Somewhere between pinch-off and the transition to the first conductance plateau, a quasibound state forms at the center of the QPC just below the Fermi energy. The quasibound state can be occupied with either a spin-up or a spin-down electron, i.e. the QPC acts as a spin-1/2 magnetic moment. The formation of the magnetic moment is accompanied by a slight rearrangement of the electron density within the QPC, which shows up as an additional dip in D .

As alluded to above, some of the present authors have performed an extensive study of the conditions under which such a magnetic moment forms in the QPC [1]. We observed this feature only in the DFT calculation within the local spin-density approximation. In the ordinary local density approximation the two spin-densities are restricted to be the same and thus spin-polarization in the QPC is not possible, while in the Hartree approximation the exchange interaction, which is responsible for spin-polarization, is absent. We observed the formation of the magnetic moment for various geometries of the QPC (rectangular shape of QPC electrodes or more adiabatic, triangular shaped electrodes) and for a wide range of QPC widths and 2DEG densities. The parameter which affects the formation of the quasibound state in the most important way is the length of the QPC. For a substantial range of QPC lengths the situation is the same as presented in this paper. However, if the QPC is very short there is not enough space for the quasibound state to form in it. If the QPC is very long an antiferromagnetically ordered spin chain forms instead of a single spin-1/2 magnetic moment.

Our present experiment cannot resolve the extra dip described by the LSDA calculation, but future, more sensitive measurements may be able to detect it.

References

- [1] T. Rejec and Yigal Meir, *Nature* **442**, 900 (2006)