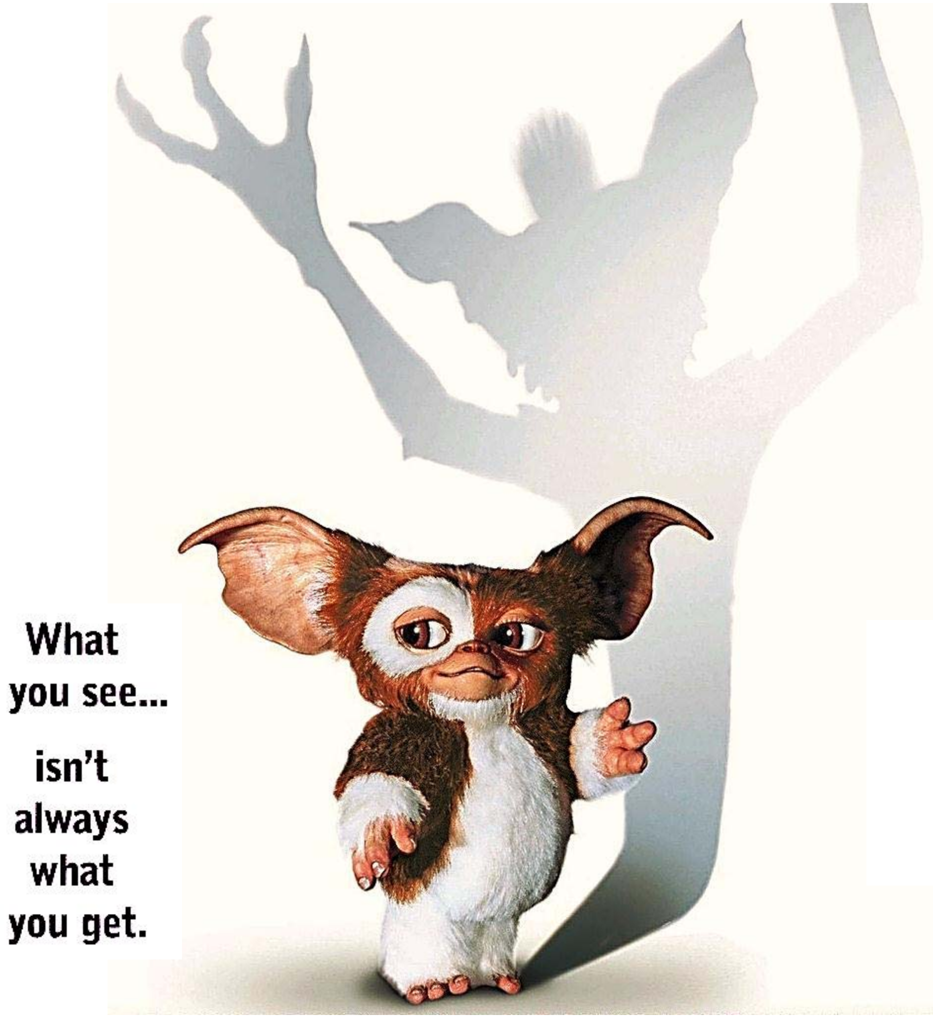
What lurks below the last plateau

15+ years of 0.7: What have we learned and where to next?



<u>Lecture 1</u>: QPCs and introduction to the 0.7 anomaly

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Your course notes…

IOP PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **23** (2011) 443201 (73pp) doi:10.1088/0953-8984/23/44/443201

TOPICAL REVIEW

What lurks below the last plateau: experimental studies of the $0.7 \times 2e^2/h$ conductance anomaly in one-dimensional systems

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Also at arXiv: 1110.3474

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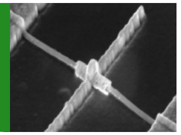


Another useful review on 1D systems

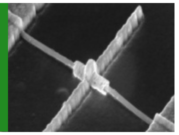
Quantum Transport in Semiconductor Nanostructures

C. W. J. Beenakker and H. van Houten

Philips Research Laboratories, Eindhoven, The Netherlands

Published in Solid State Physics, 44, 1-228 (1991)

Contents



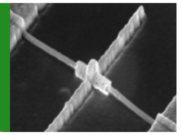
A rough breakdown of the course…

Lecture 1: Recap on the physics of QPCs and 1D systems, measuring 1D subband spacing and *g*-factors, introduction to the 0.7 anomaly, initial observations and initial theoretical support from density functional theory.

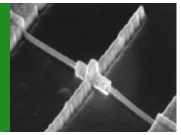
Lecture 2: The Bruus-Cheianov-Flensberg and Reilly models, thermal activation studies, shot noise, density dependence of 0.7, the 0.7 analogs and complements, subband tracking experiments, Moving beyond phenomenological models.

Lecture 3: The Kondo effect in metal films and quantum dots, smoking guns and scaling, Kondo in QPCs, bound states in theory calculations, deliberately inducing bound states, further studies of Kondo in QPCs, Kondo and holes.

Lecture 4: Bound state controversy, the Fano effect, Fano resonance studies in mesoscopic devices and coupled QPCs, more complex spontaneous ordering of electrons – theory and experiment, the edge of knowledge, the disorder problem.

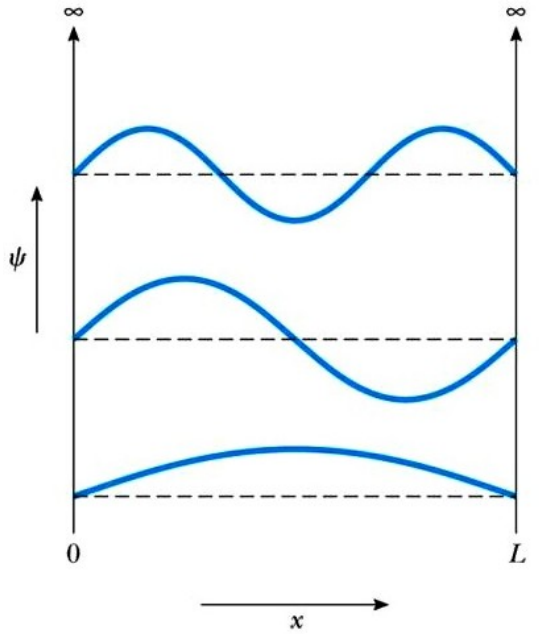


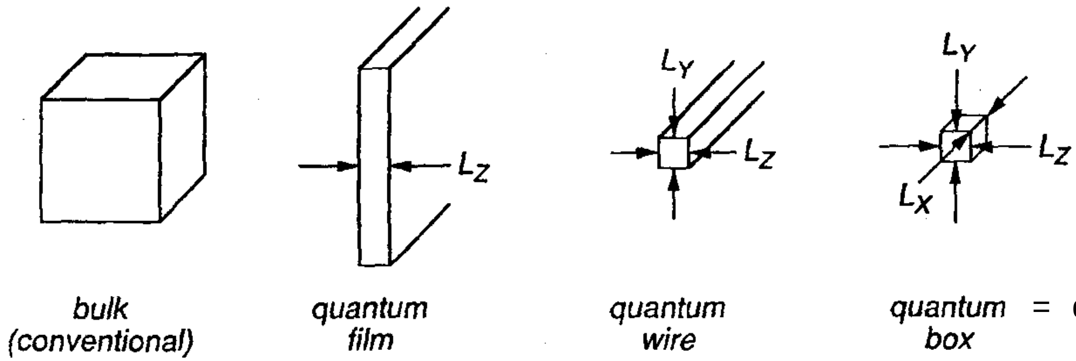
Introduction: A recap on QPCs



Reducing dimensions

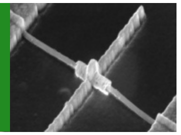
- **We can now make semiconductor structures sufficiently small that they are of the order of the electron wavelength.**





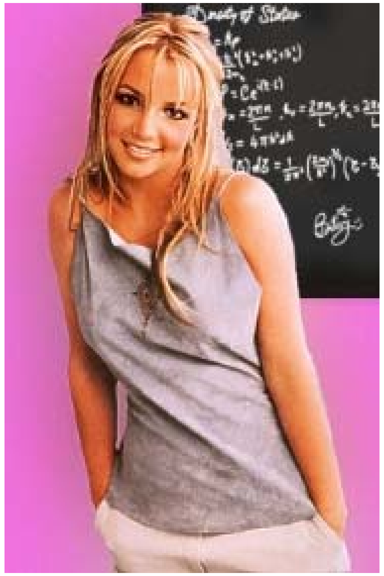
= quantum dot

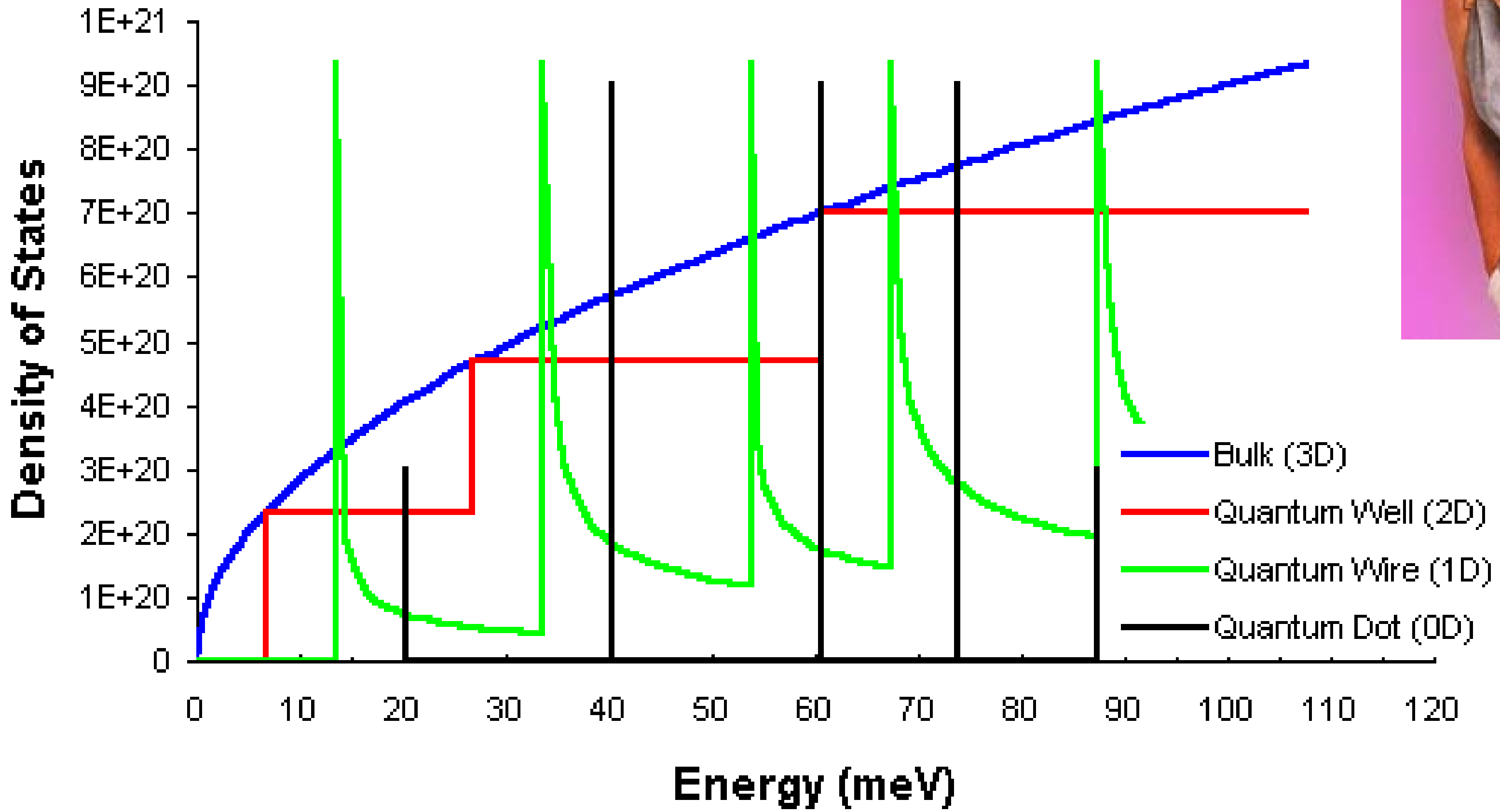
- **This allows us to study very fundamental quantum mechanical systems, such as the classic ‘particle in a box’ problem.**

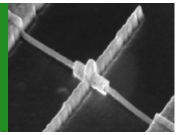


Densities of States: 3, 2, 1 and 0D

See http://britneyspears.ac/physics/dos/dos.htm for full details

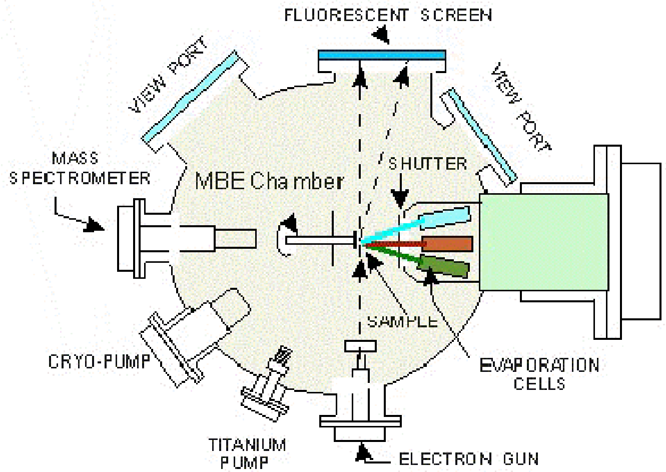


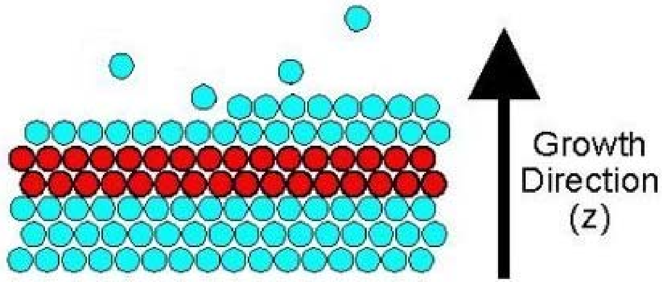




Making low-dimensional systems

- **Part of the magic is having control over materials at the atomic level.**





- **Molecular beam epitaxy (MBE) lets you grow materials one atomic layer at a time, and make very thin layers of materials sandwiched between other layers.**

You can take this sort of control a long way…

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Kvantdatorer – mer än ettor och nollor

FOTO: GUNNAR LUNDMARK, TORSTEN BLACKWOOD/AFP, SCANPIX

KTH, som i september presenterade en ny superdator som kommer att bli den mest kraftfulla i Norden, är ett av universiteten som forskar om kvantdatorer. I maj i år visade professor Michelle Simmons på centrum för kvantdatorteknik vid University of South Wales i Australien upp en kvanttransistor som kan bli en hörnsten i kommande kvantdatorer. Transistorn är endast sju atomer bred. En kvantdator kan få enormt mycket större beräkningskapacitet än traditionella datorer och därmed ha stor betydelse för bland annat läkemedelsforskning. Nobelpristagaren Richard Feynman talade om kvantsystem redan på tidigt 1980-tal.

Kvantdatorer – mer än ettor och nollor

INNOVATION | En dator så liten att den inte syns

Publicerad: 4 oktober 2010, 08.00. Senast ändrad: 4 oktober 2010, 08.18

Om mindre än tio år kan vi ha en ny typ av datorer som blir enormt mycket mer kraftfulla än dagens. Det hävdar brittiska forskare sedan de utvecklat ett chip som öppnar en ny väg mot kvantdatorer. Men utmaningarna är enorma och andra forskare varnar för att det snarare tar 30 år till, om det nu alls blir verklighet.

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- 07:40 E24 Axfood höjer vinsten
- 07:31 E24 Årshögsta i Oslo efter miljardaffär
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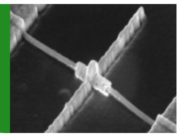
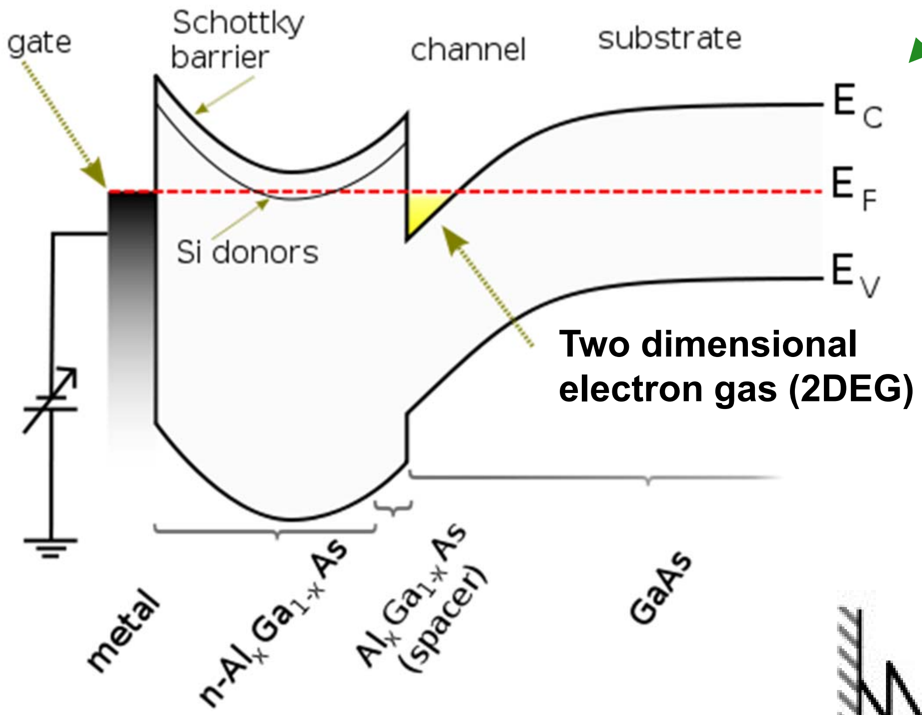
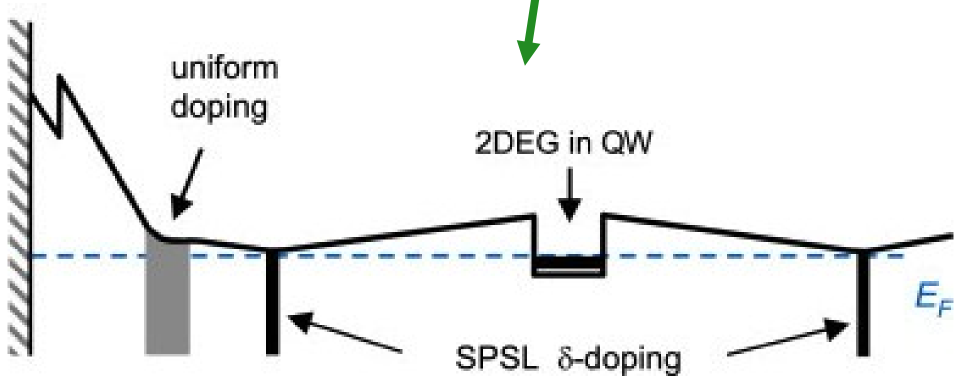


The confinement in a 2D well – HJs and QWs

- **Two common ways to achieve a 2DEG – A heterojunction and a quantum well.**

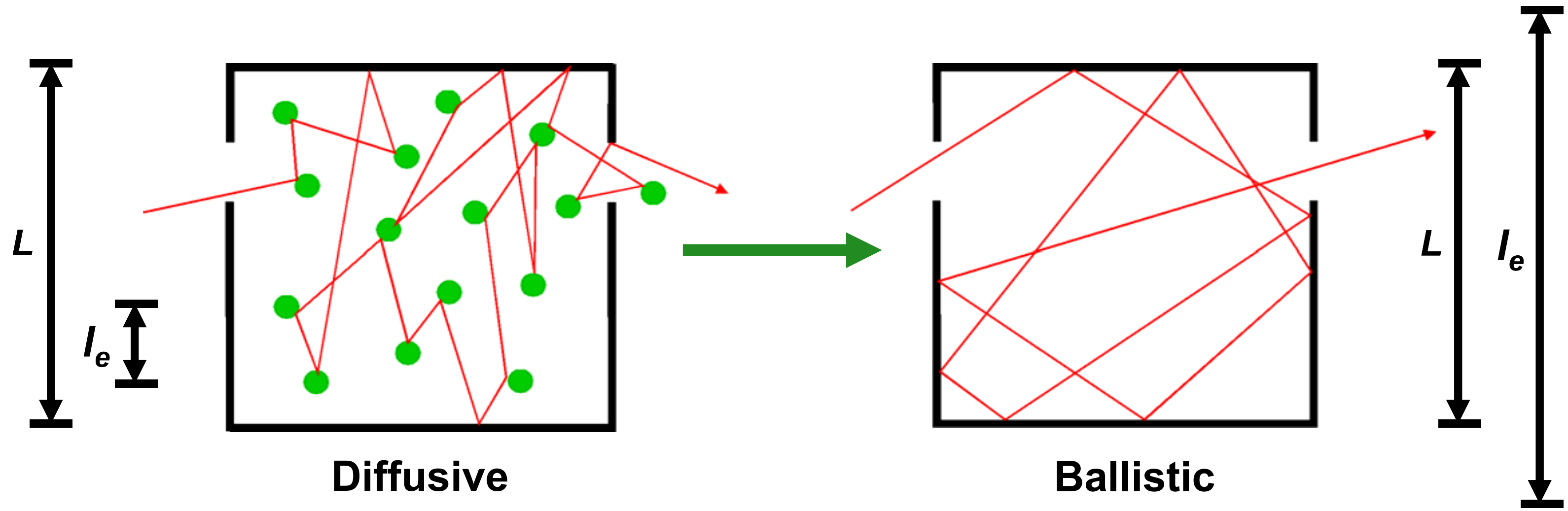




Ballistic transport (for now…)

- Low mobility devices – diffusive transport, trajectory largely determined by random impurity distribution.

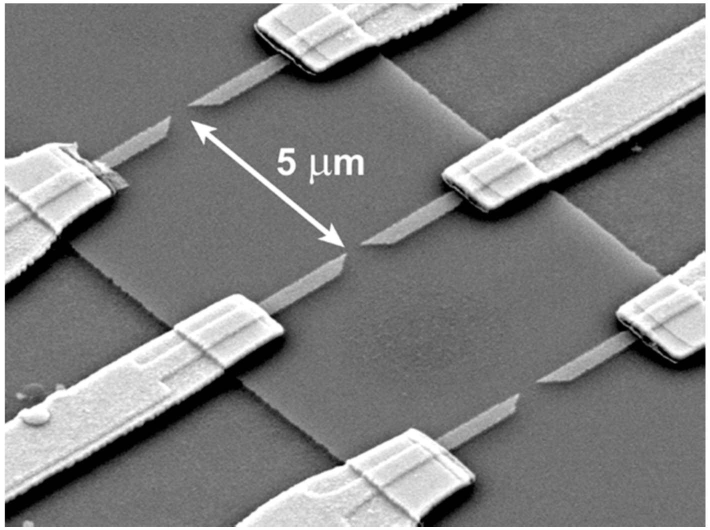
- High mobility devices – ballistic transport, trajectory largely determined by reflection of structures

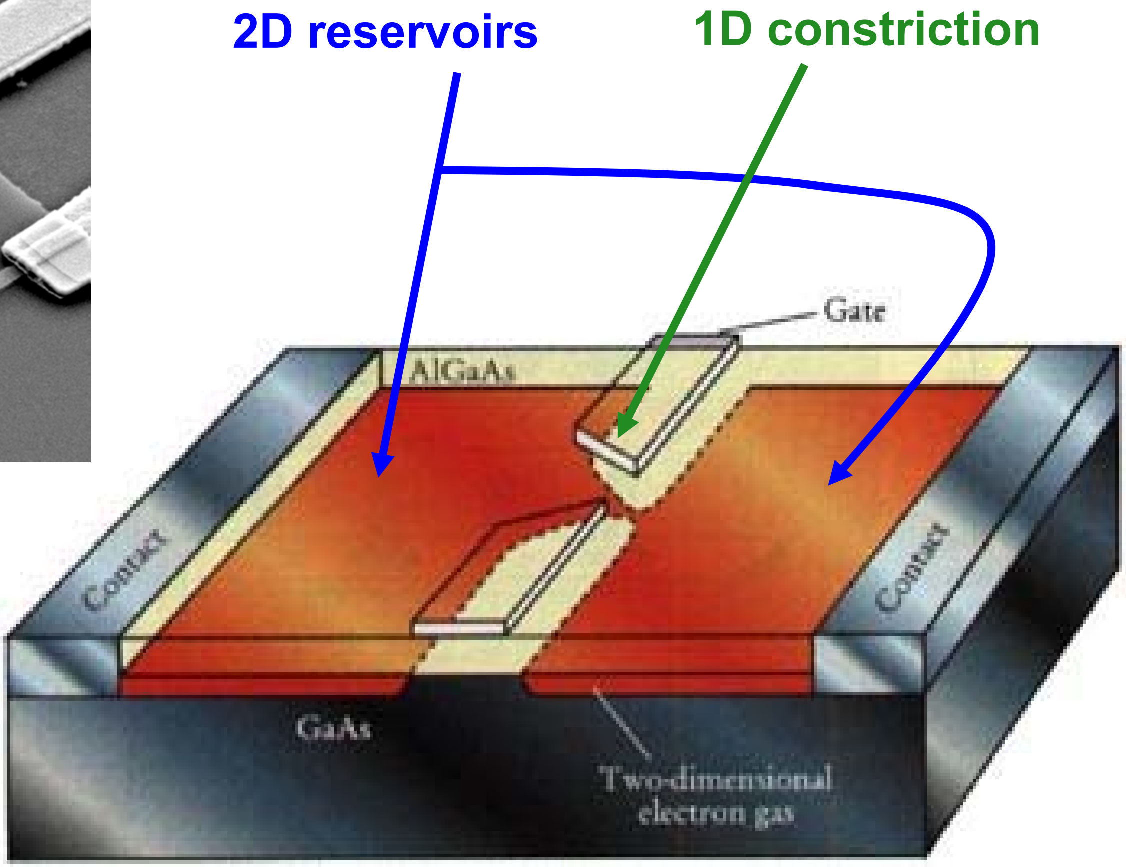


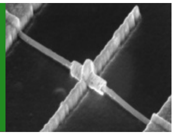
- Conductance quantization in QPCs can only be observed in the ballistic regime.

Making 1D - The Quantum Point Contact (QPC)

- It is fairly easy to realise a 1D system. It is typically done using the ‘split gate’ technique.

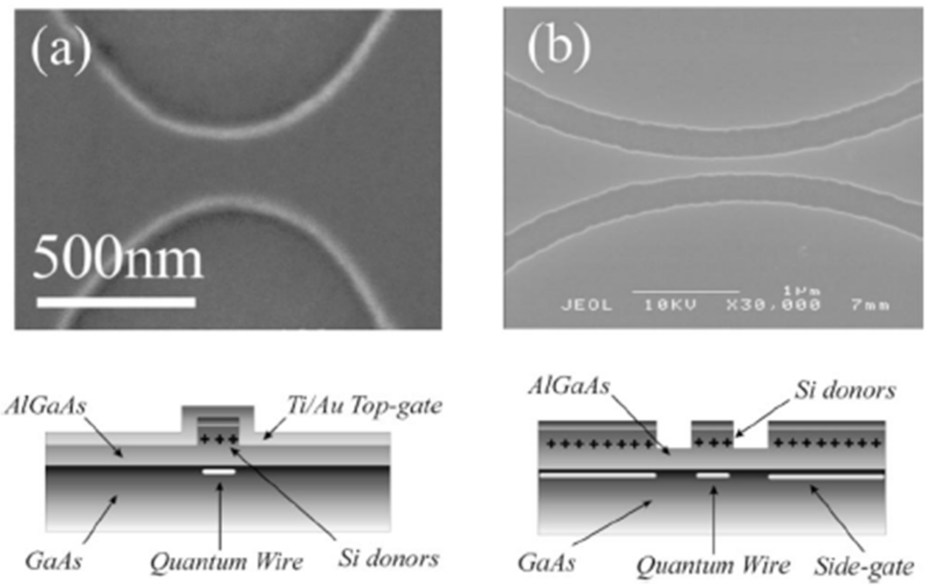




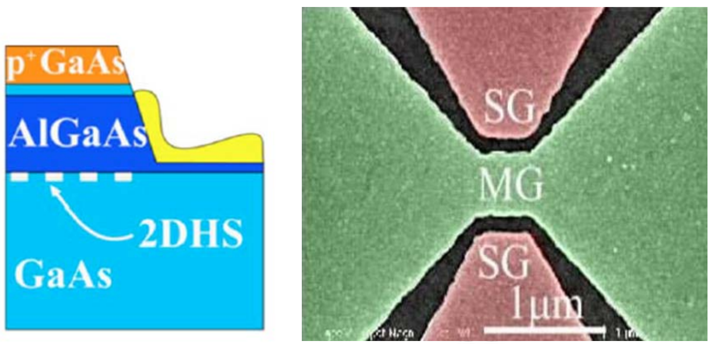


Other ways for making QPCs

Etching

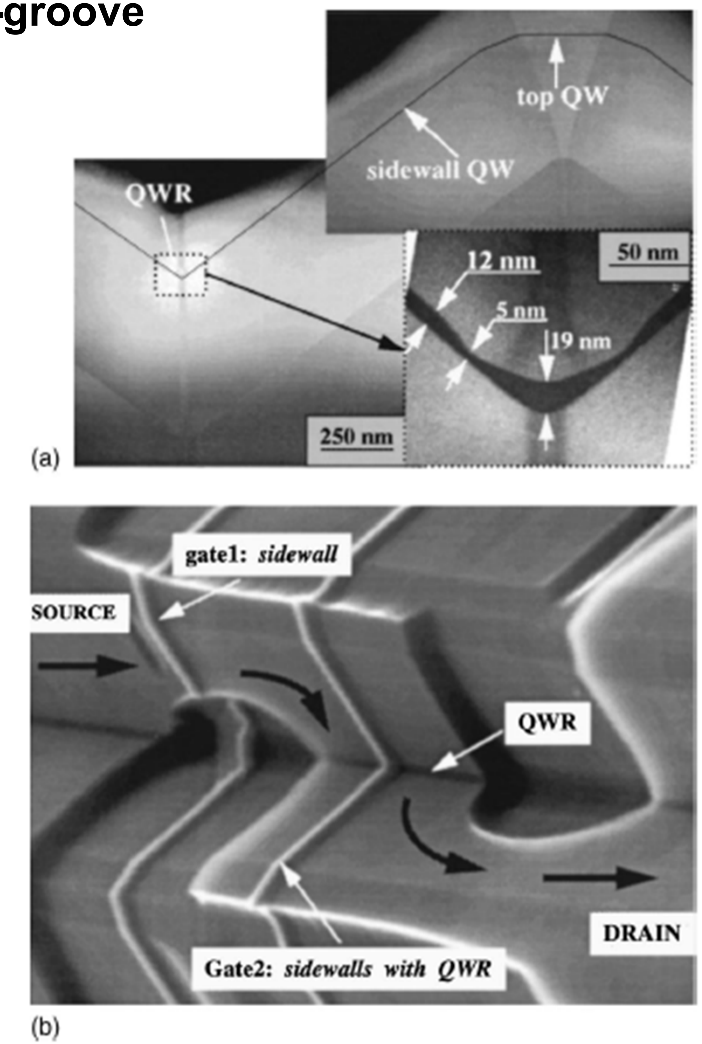


A. Kristensen *et al.*, PRB <u>62</u>, 10950 (2000).

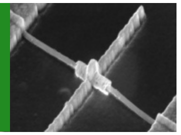


O. Klochan *et al.*, APL <u>89</u>, 092105 (2006).

V-groove

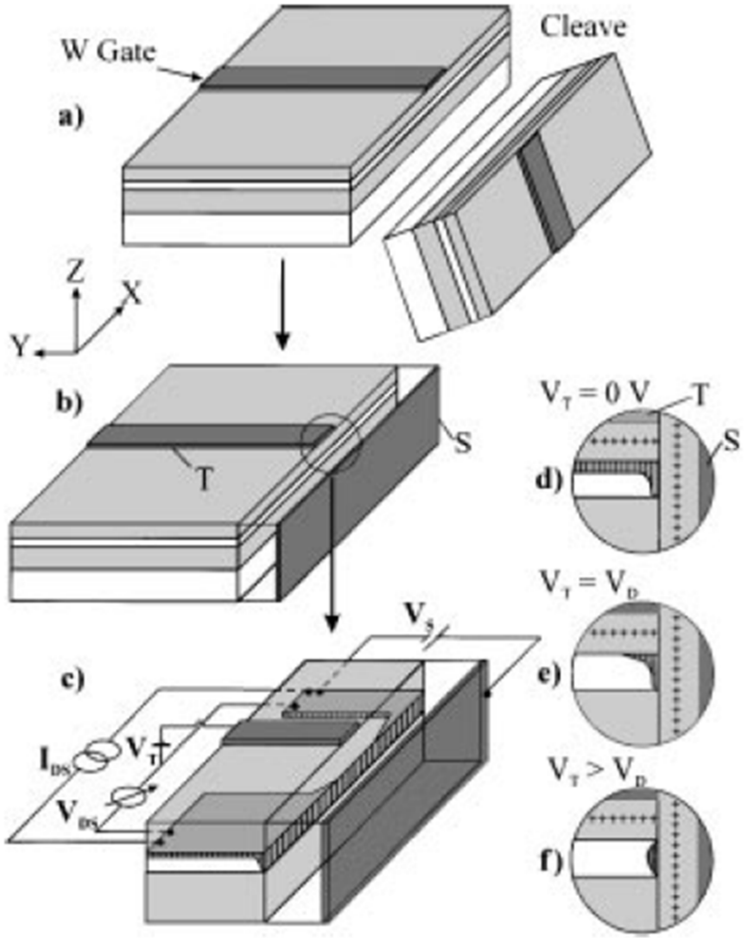


D. Kaufman *et al.*, PRB <u>59</u>, R10434 (1999).



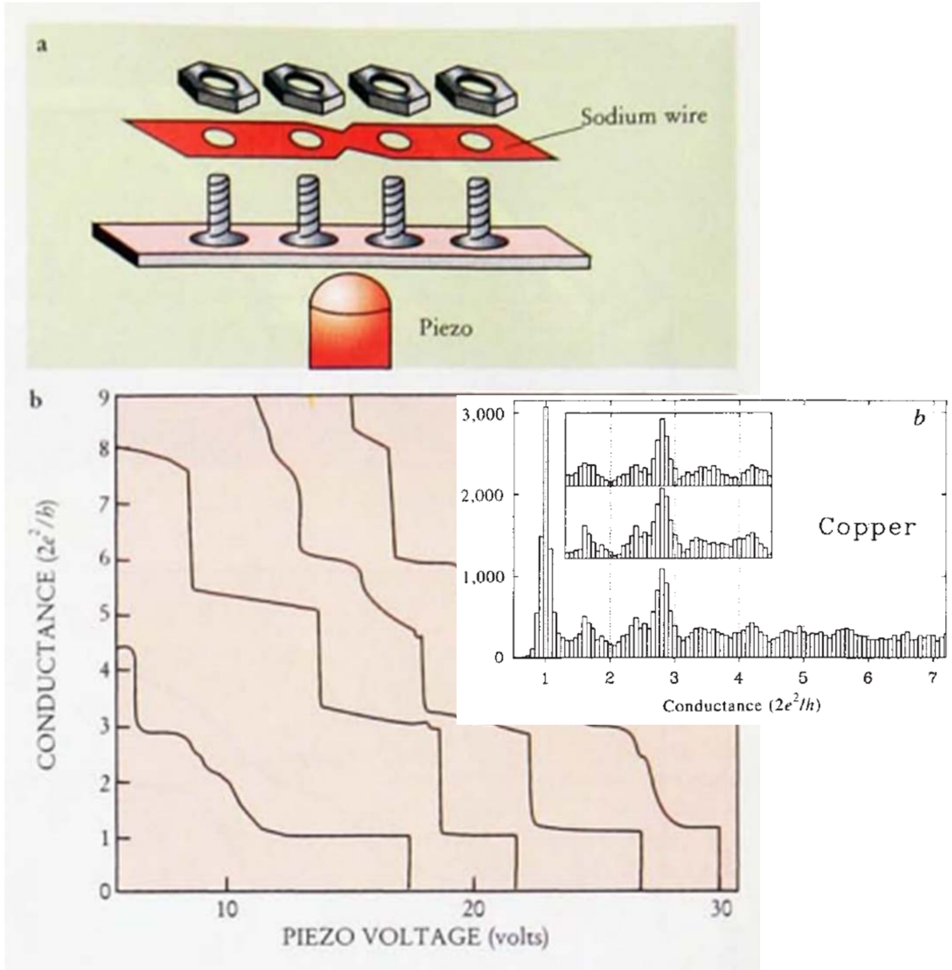
Other ways for making QPCs

Cleaved edge overgrowth



A. Yacoby *et al.*, PRL 77, 4612 (1996).

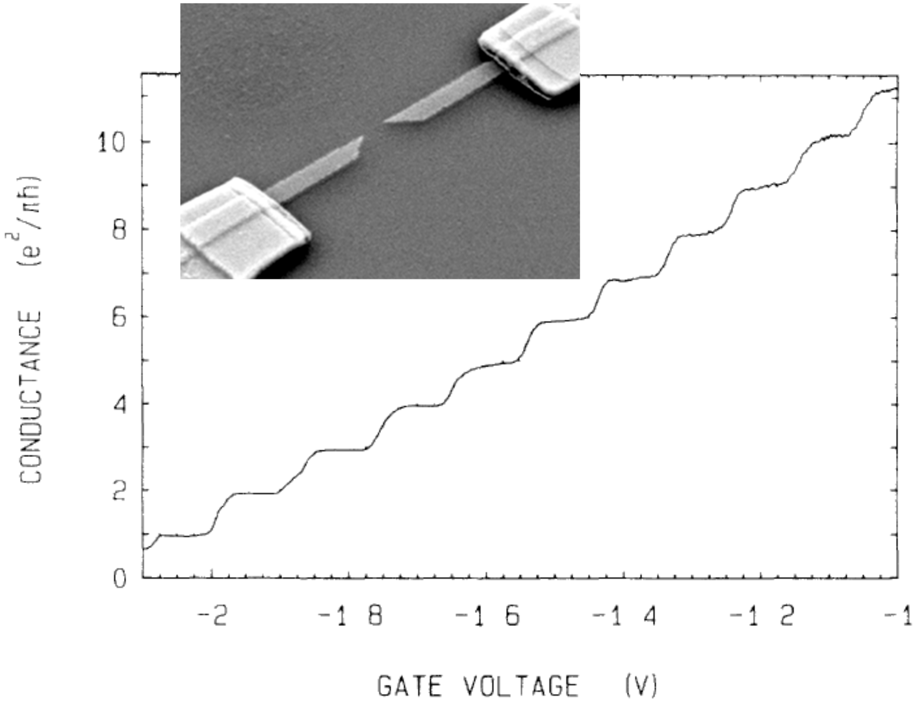
Metallic Break Junctions

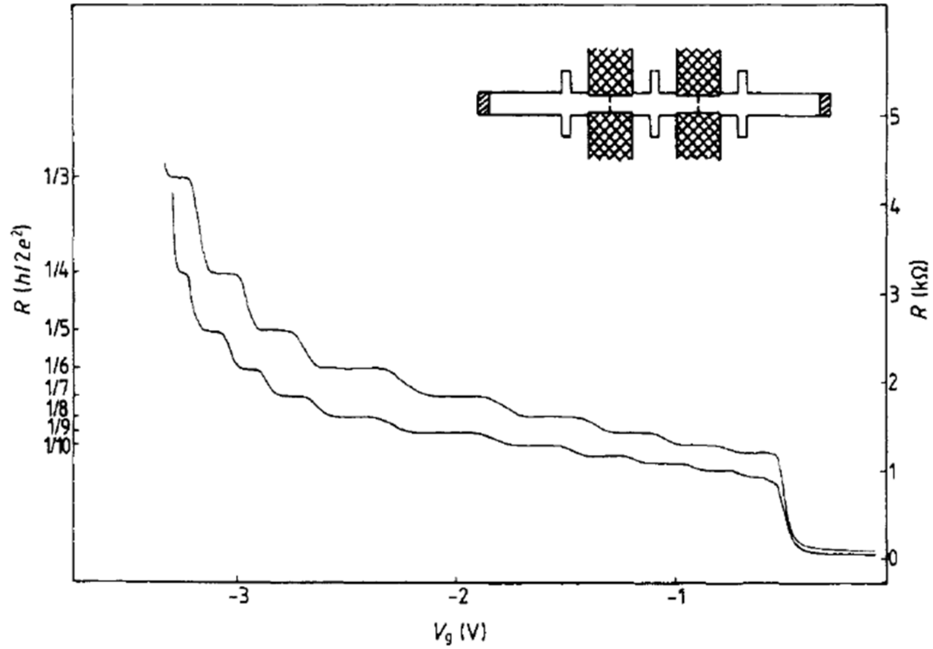


J.M. Krans *et al.*, Nature 375, 767 (1995).

Homage to Wharam and van Wees

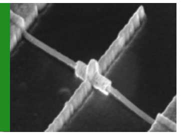
- **It will be 25 years since these results in January/February next year.**





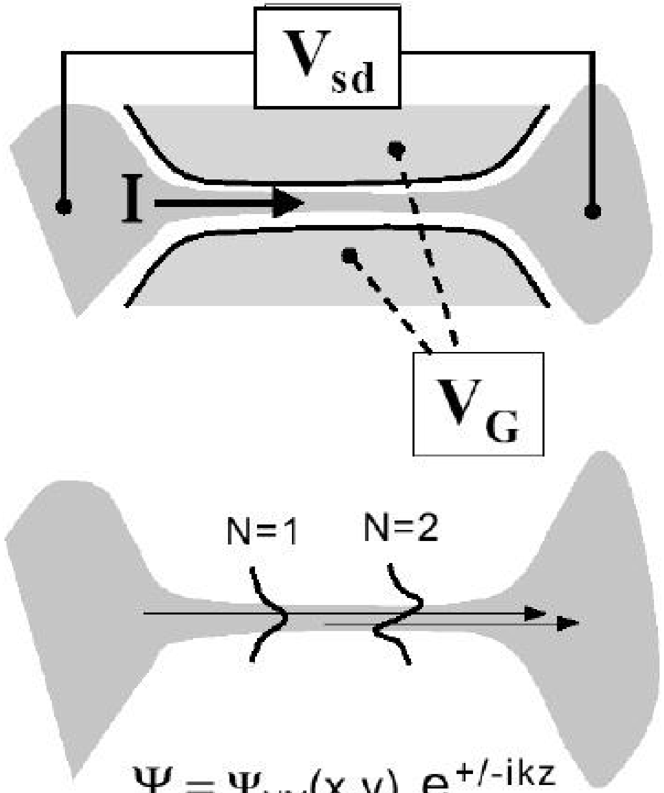
B.J. van Wees *et al.*, PRL <u>60</u>, 848 (1988).

D.A. Wharam *et al.*, J. Phys. C <u>21</u>, L209 (1988).



The waveguide analogy

- **In many respects, a QPC or 1D channel is just a waveguide.**



$\Psi = \Psi_{NM}(x,y)\ e^{+/-ikz}$

Transmission of one mode:

$$w = n\frac{\lambda_F}{2}$$

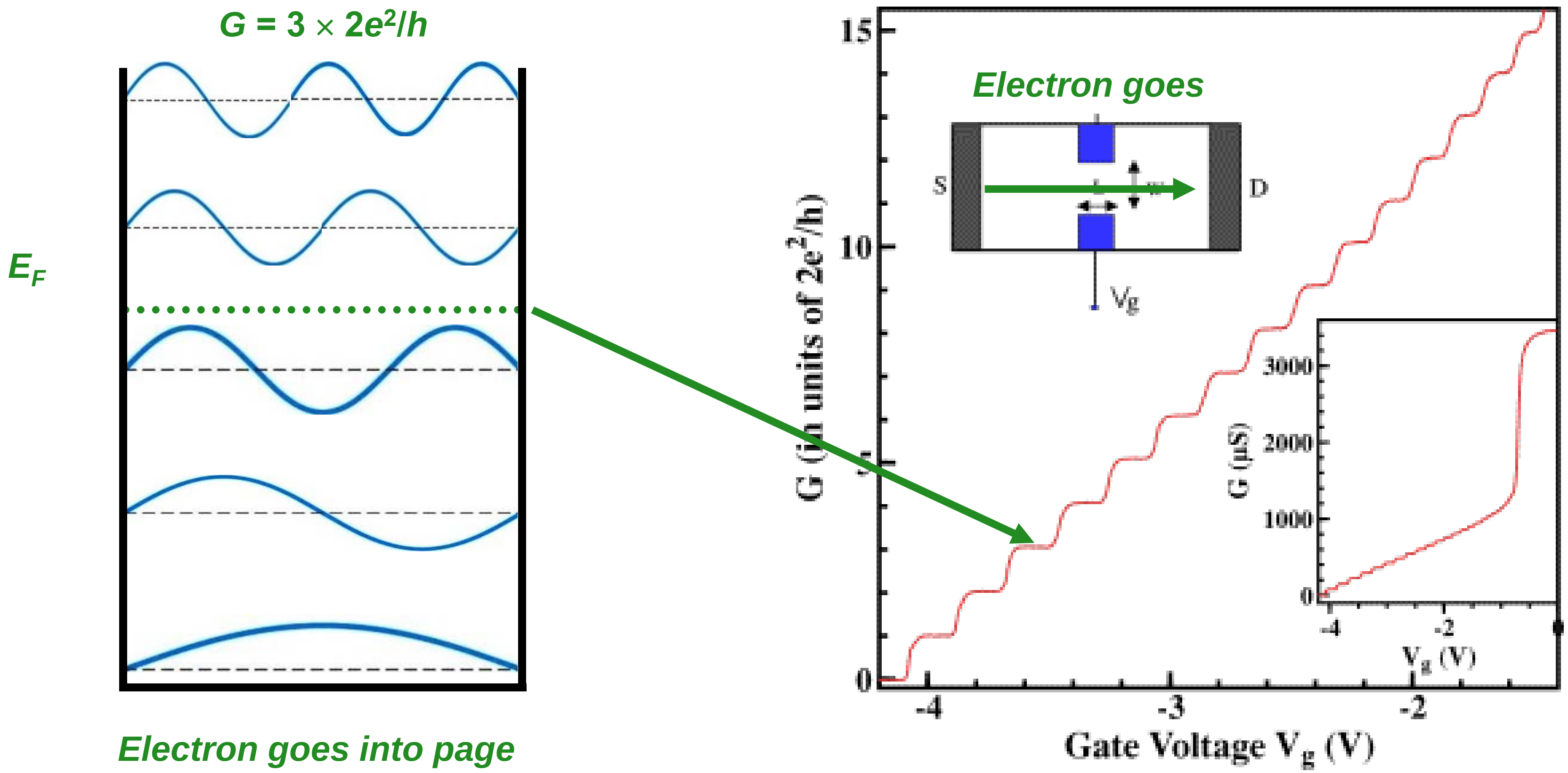
$$G = 2\frac{e^2}{h}\mathrm{Int}\left[\frac{w}{\lambda_F/2}\right]$$

1st mode transmitted for $w = \lambda_F/2$

2nd mode transmitted for $w = \lambda_F$

Quantization of 1D conductance

- **If you measure the conductance through the wire as a function of the voltage applied to the two gates defining it, you see a set of steps in the conductance.**



- **This occurs because as you increase the voltage, you decrease the width of the wire *L*, which pushes the energy eigenvalues up above the Fermi energy one by one.**

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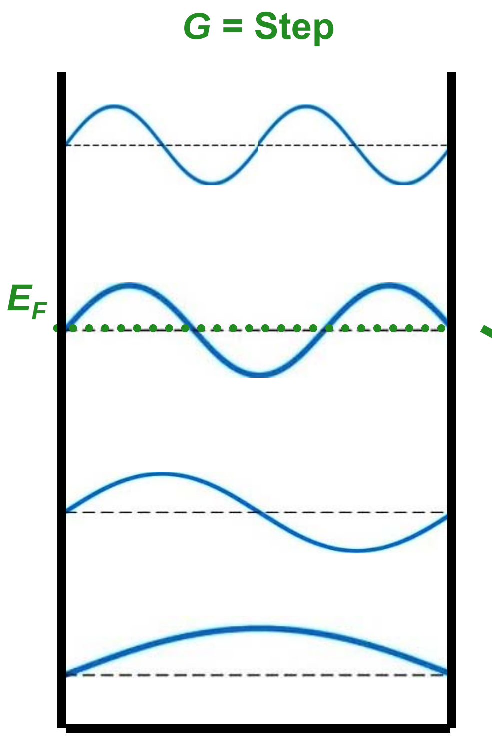

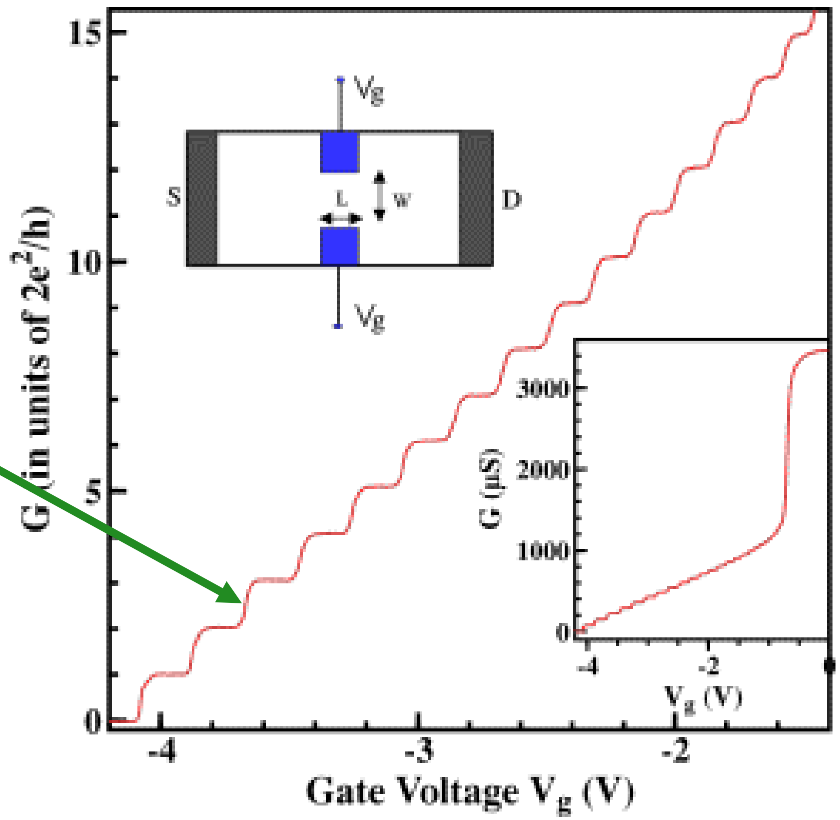

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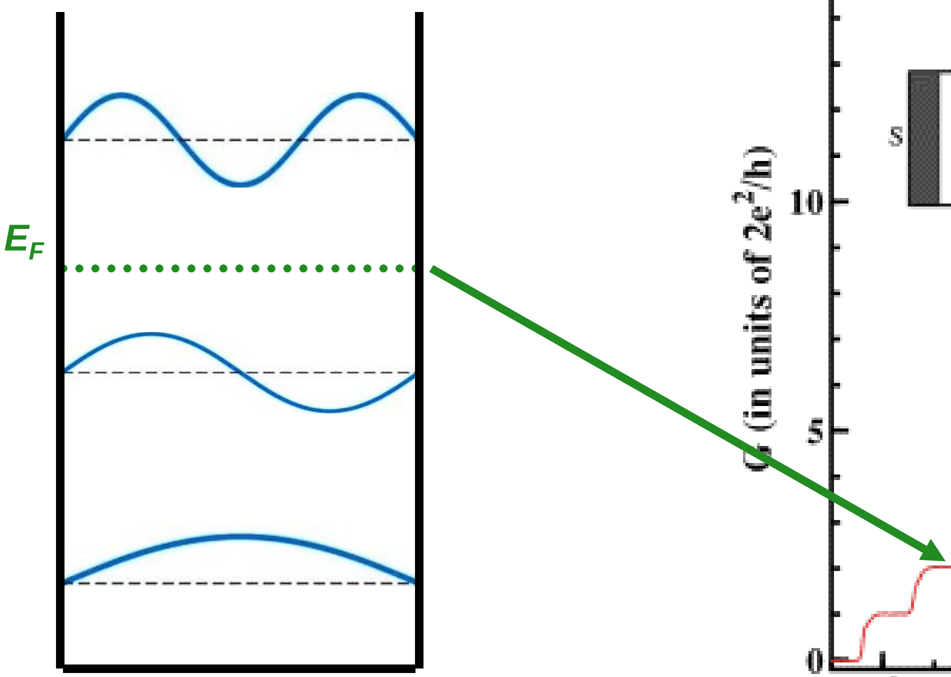

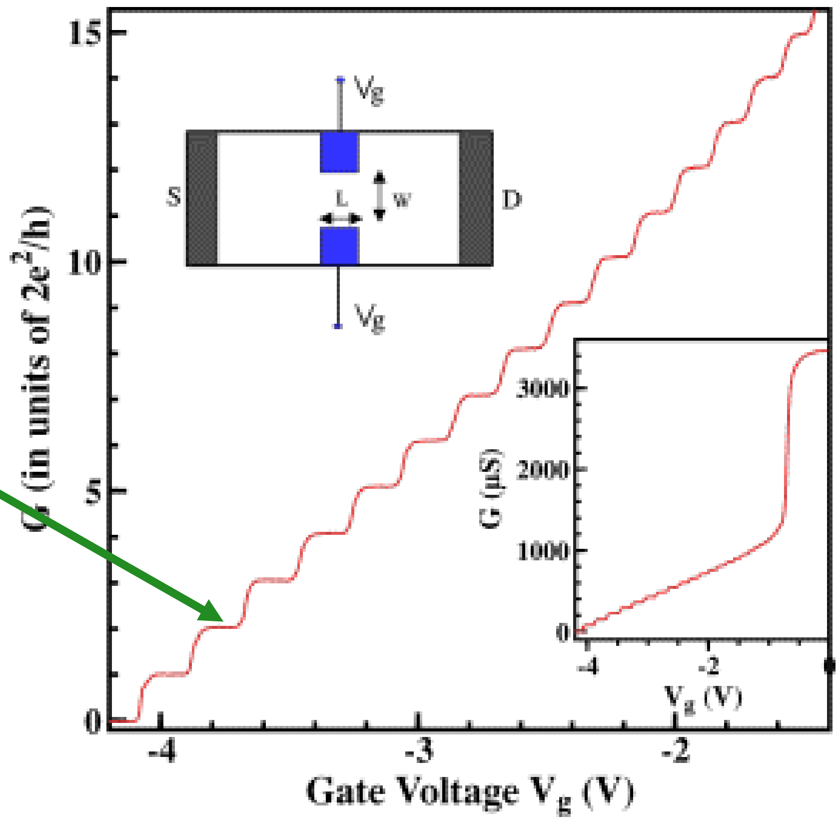

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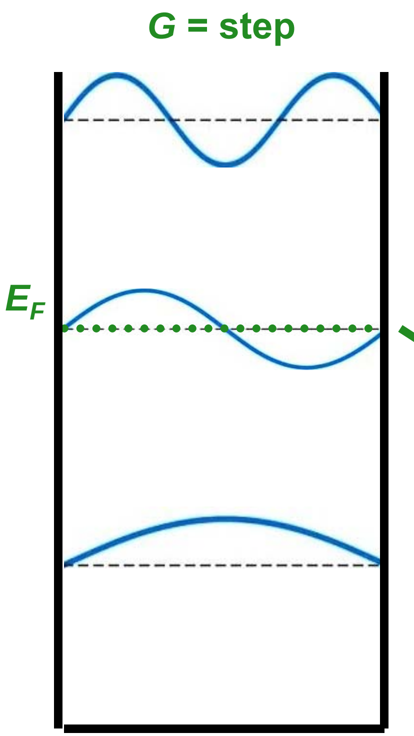

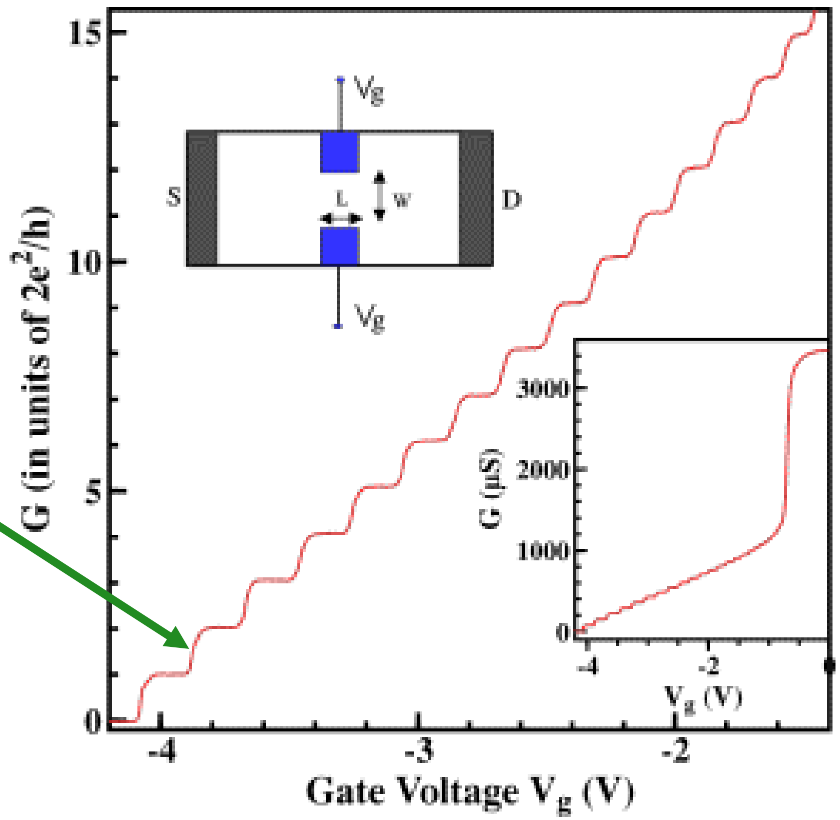

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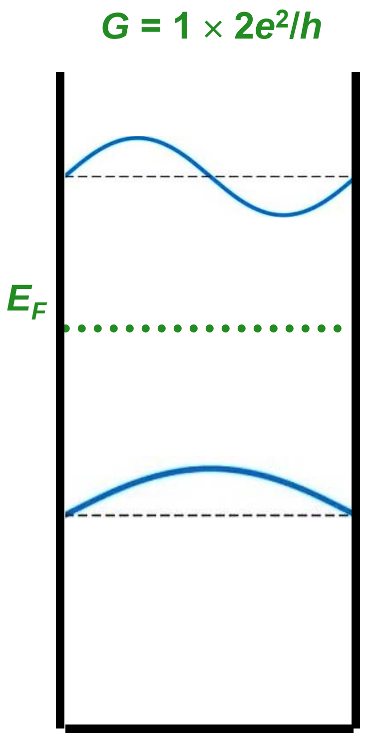

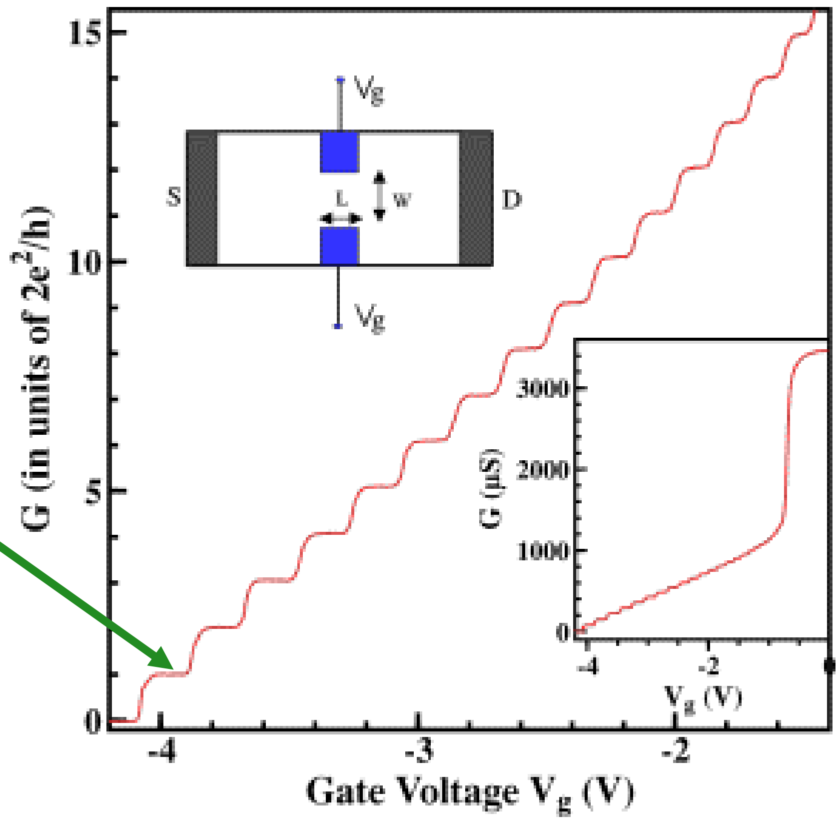

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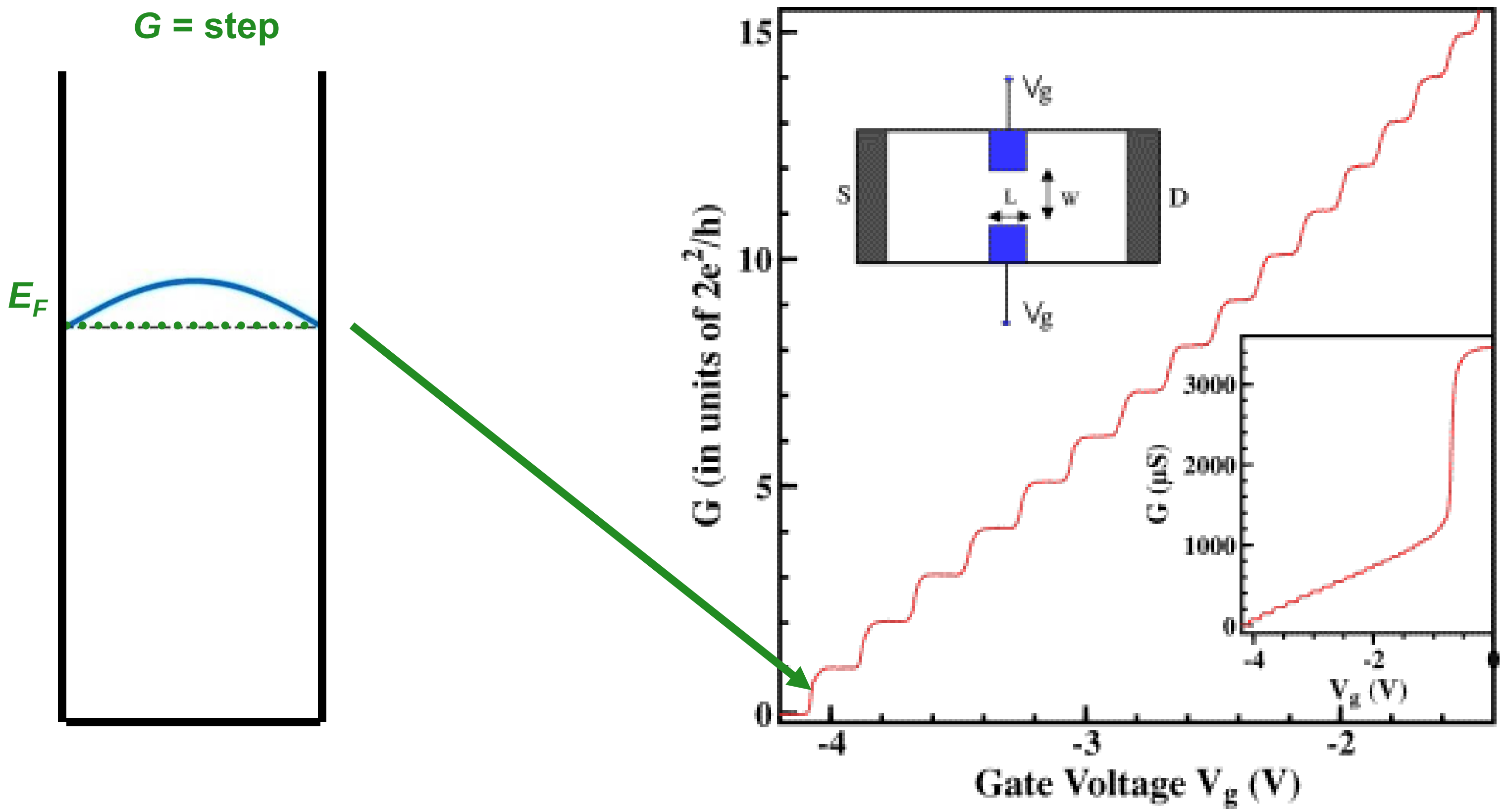

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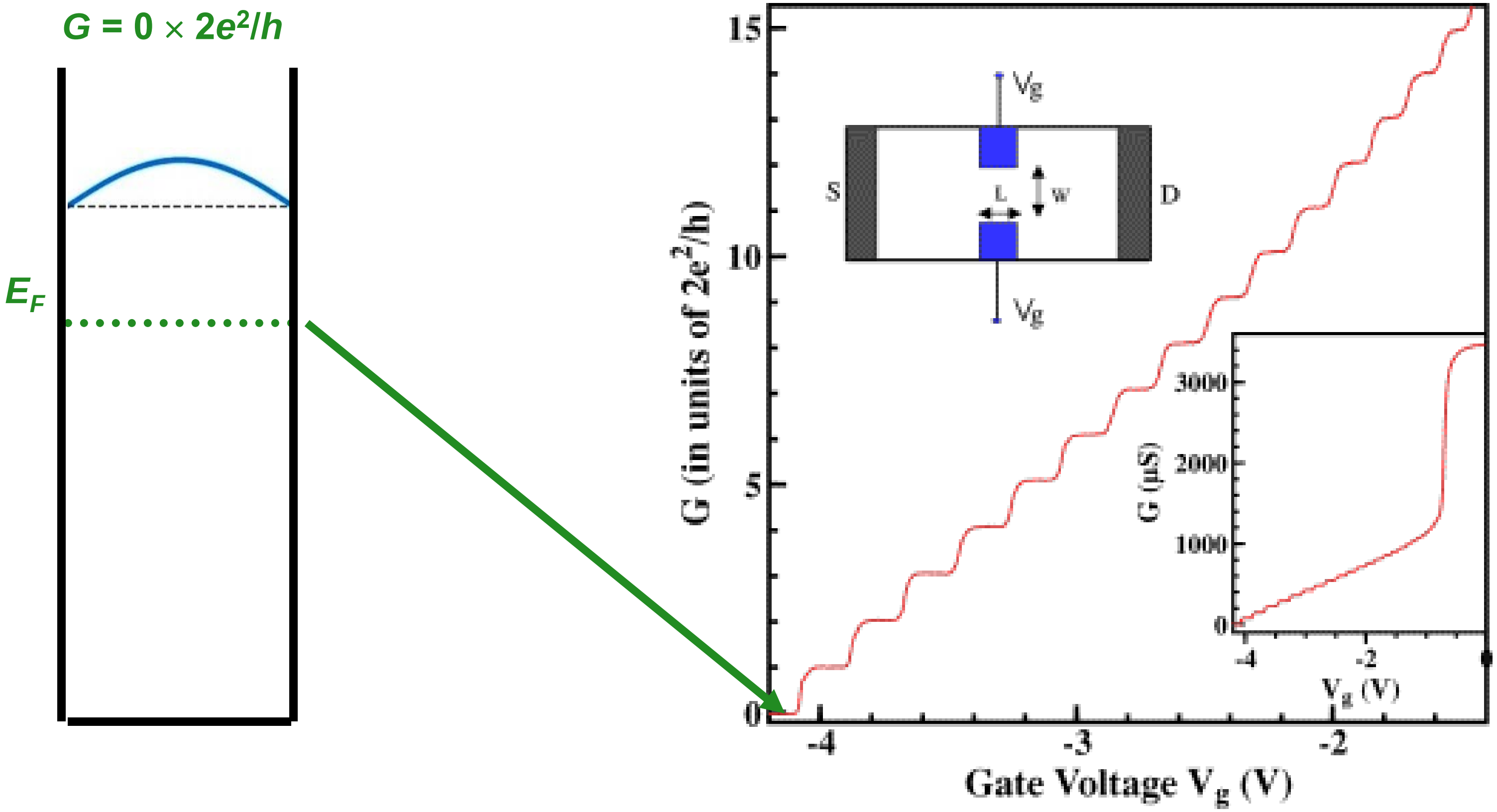

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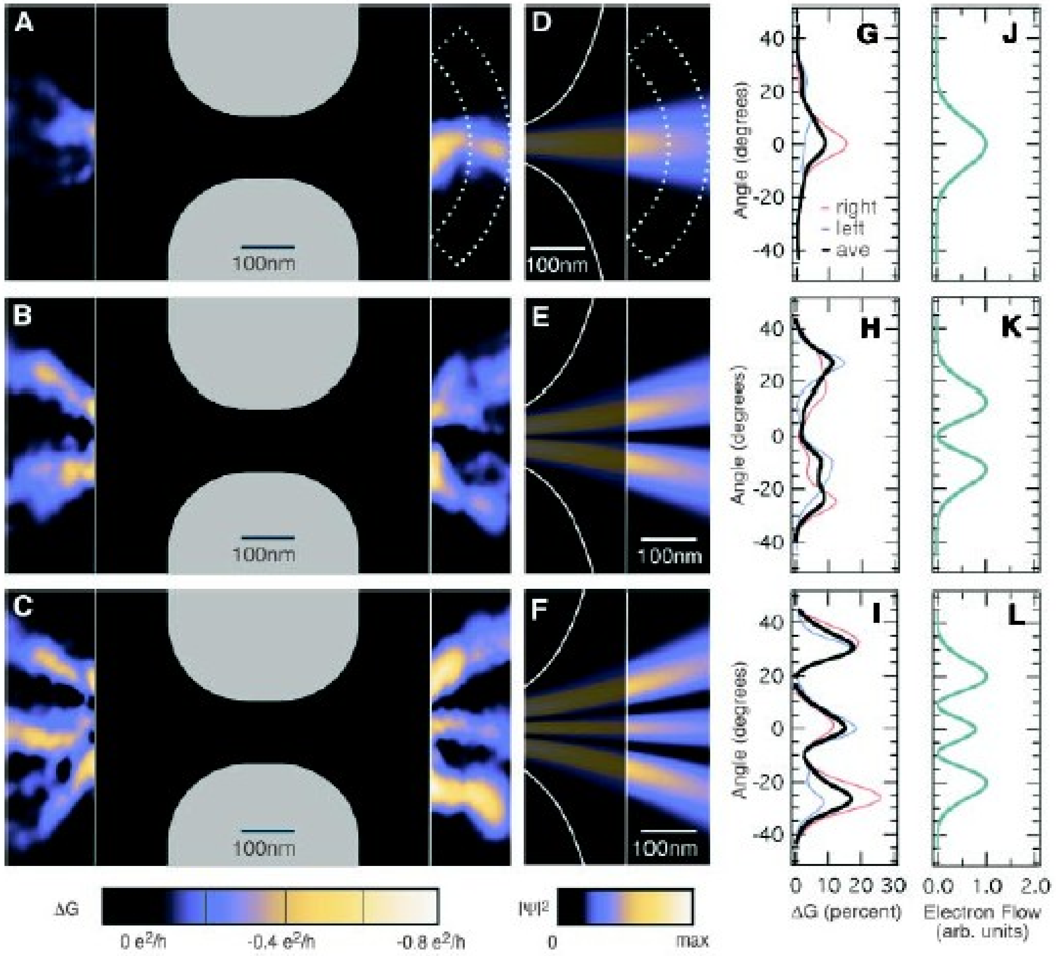
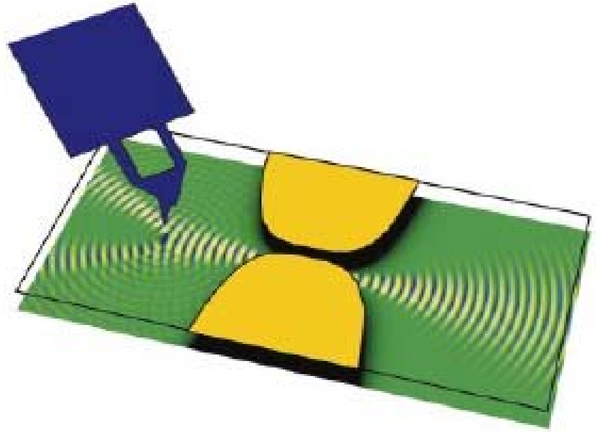
A QPC's mode structure is observable

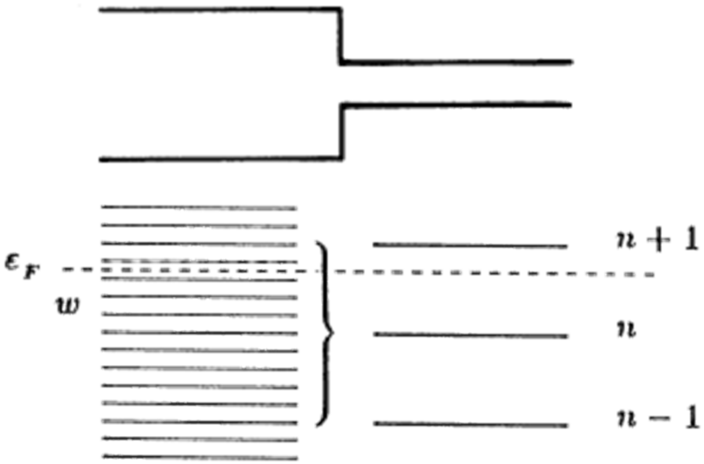


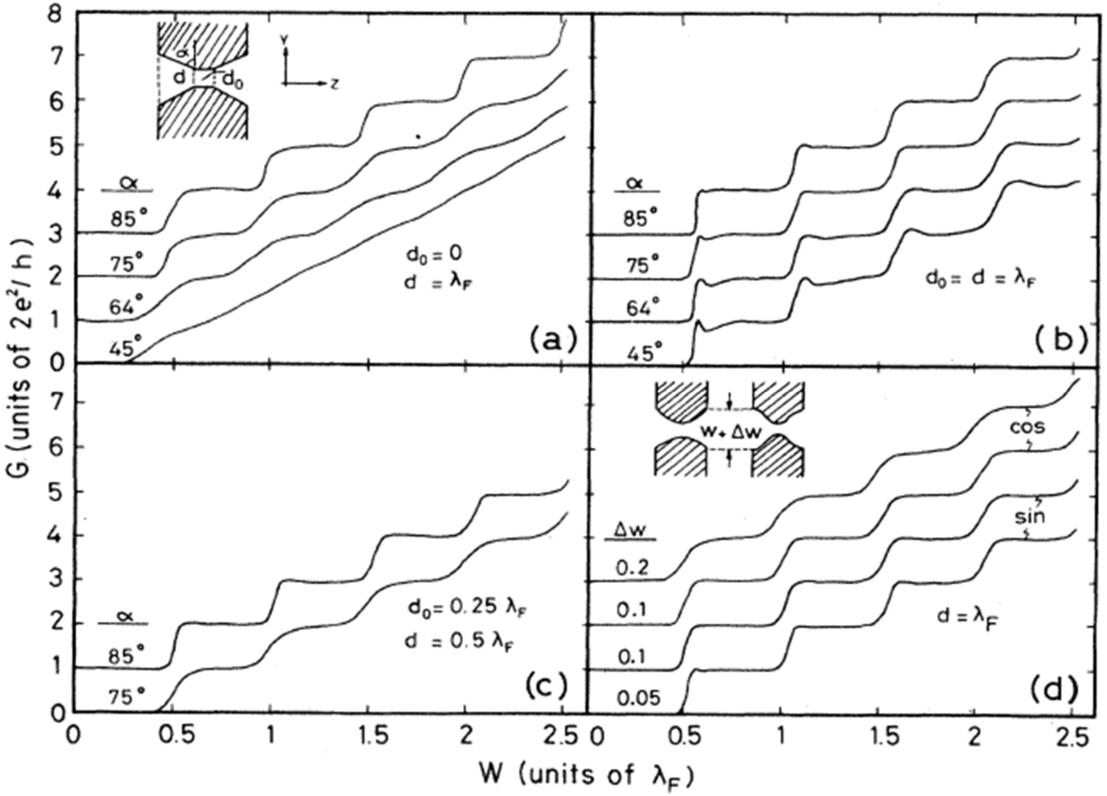


M. Topinka *et al.*, Science 289, 2323 (2000).

How do these steps compare to QHE plateaus?

- **The plateaus are not perfectly quantized nor are they perfectly sharp steps. This is partially due to disorder, but also partially due to mode-matching effects.**





Glazman *et al.*, JETP Lett 48, 238 (1988); Szafer & Stone, PRL 62, 300 (1989); Tekman & Ciraci, PRB 40, 8559 (1989).

Why is the conductance quantized at all?

- **Energy terms in the density of states and the electron velocity conveniently cancel to give a quantized conductance.**

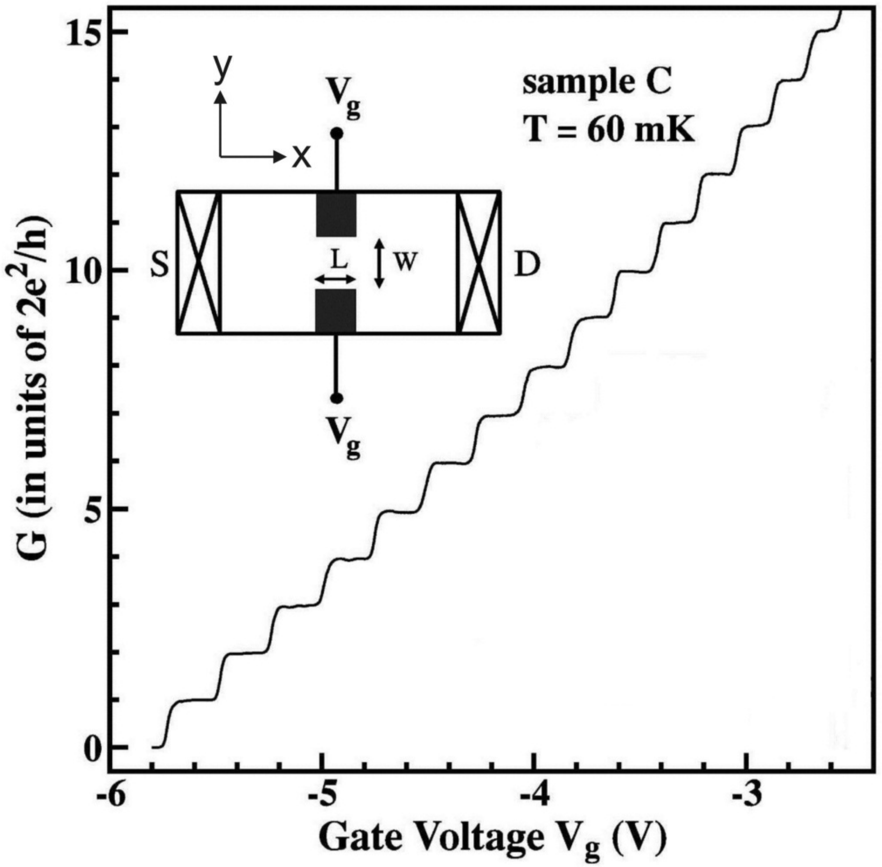
$$I = \int_0^{E_F} n_{1D}(E)\, e\, v(E)\, dE$$

$$n_{1D}(E) \propto 1/\sqrt{E},$$ 1D density

and $v(E) \propto \sqrt{E},$ Electron velocity

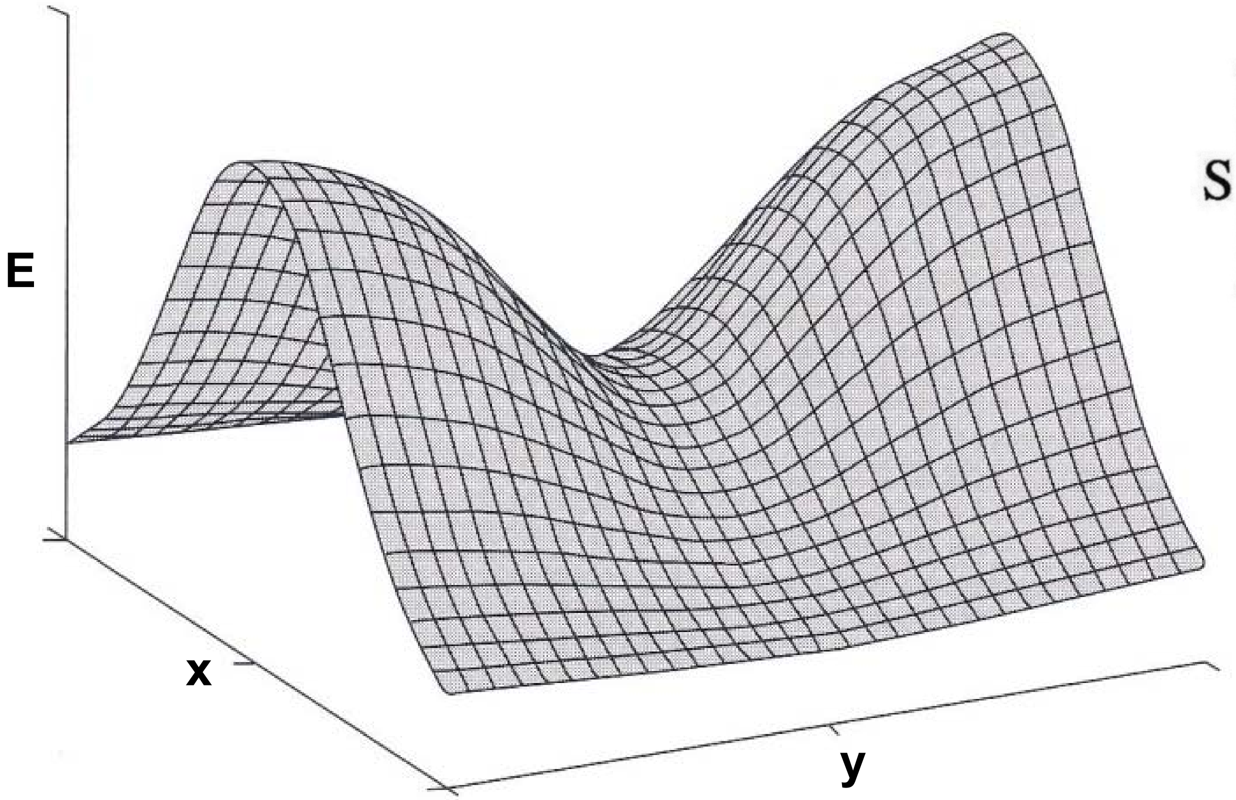
so $I = \dfrac{2e^2}{h} V$

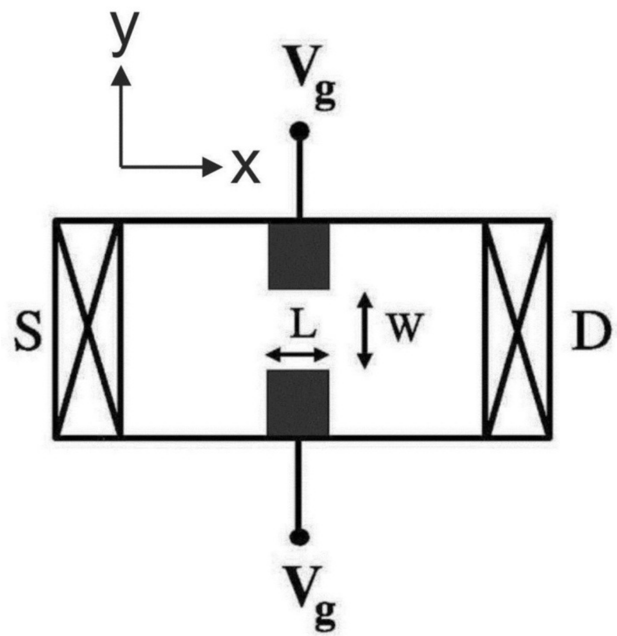
$$\frac{I}{V} = \frac{1}{R} = G = \frac{2e^2}{h}$$



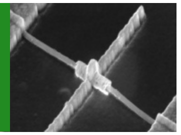
The saddle-point potential

$$V(x,y) = V_0 - \frac{1}{2} m\omega_x^2 x^2 + \frac{1}{2} m\omega_y^2 y^2$$

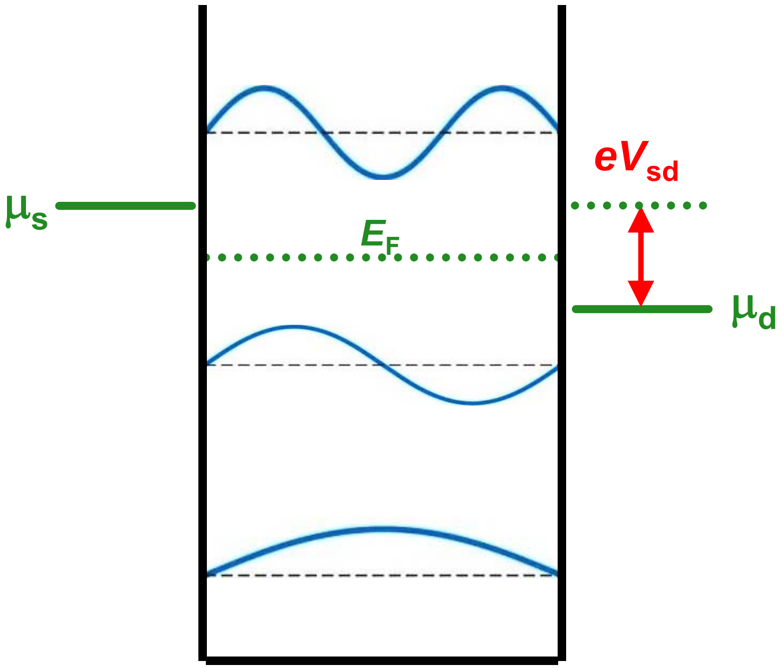


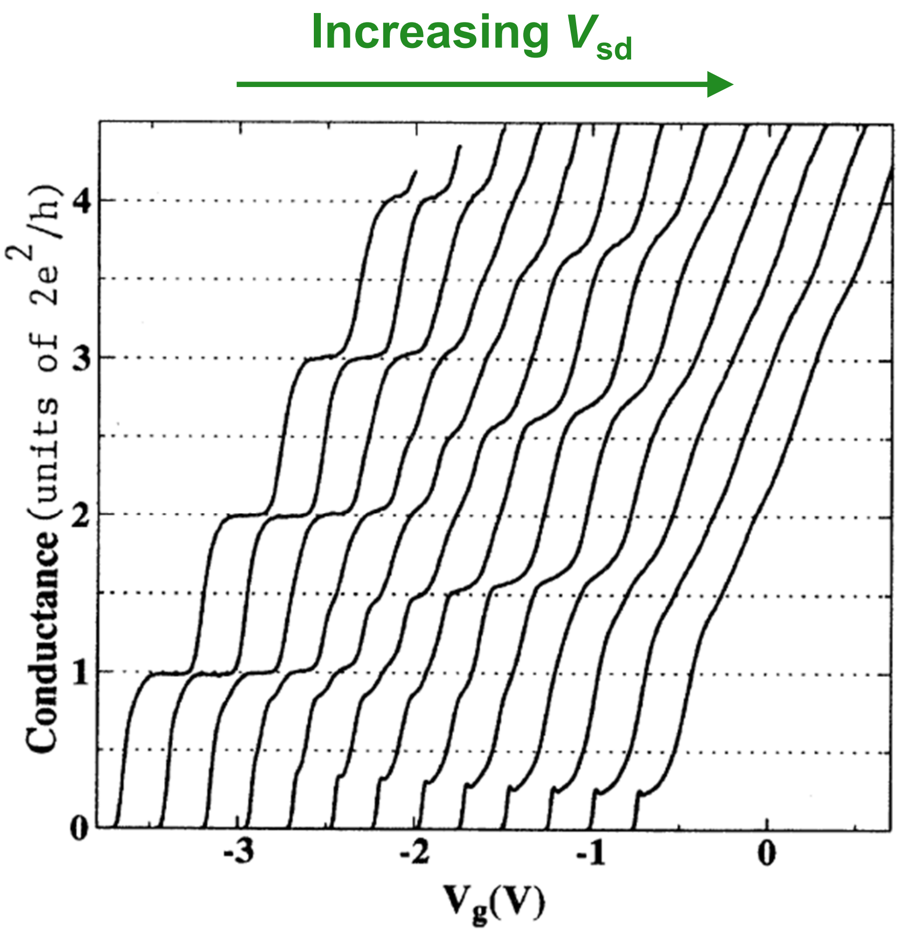


M. Büttiker, PRB 41, 7906 (1990).



1D plateaus under a source-drain bias

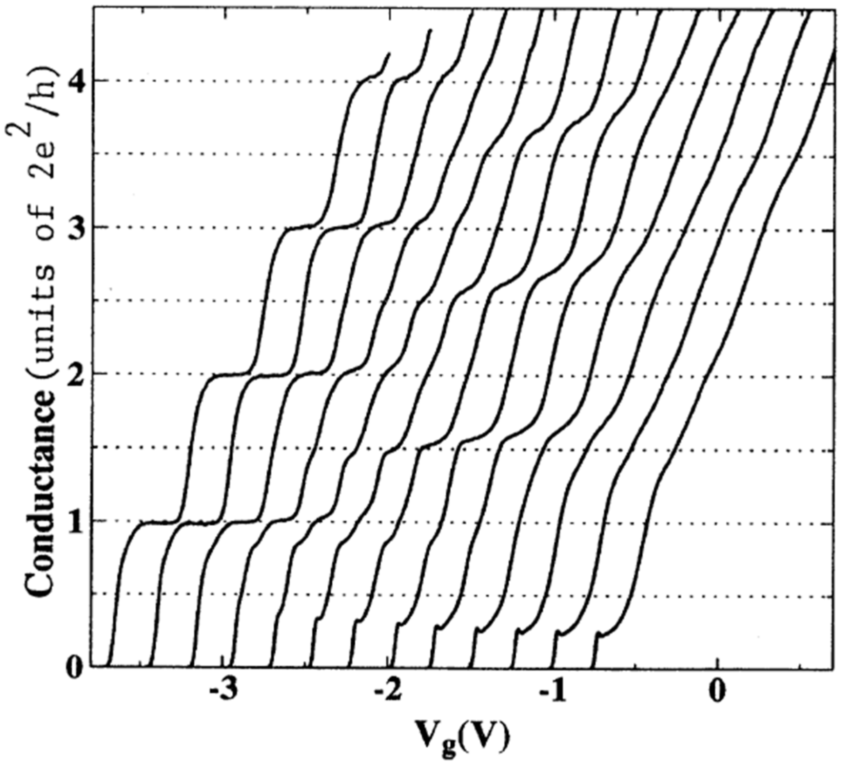


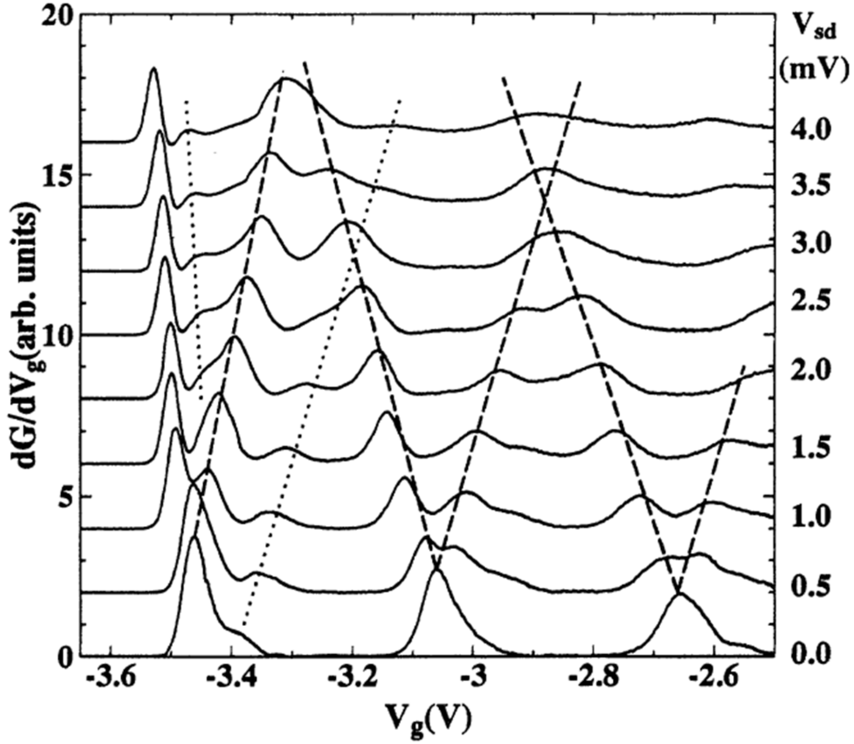


N.K. Patel *et al.*, PRB 44, 13549 (1991).

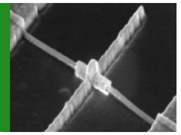
Measuring the 1D subband spacing

Increasing V_{sd} →

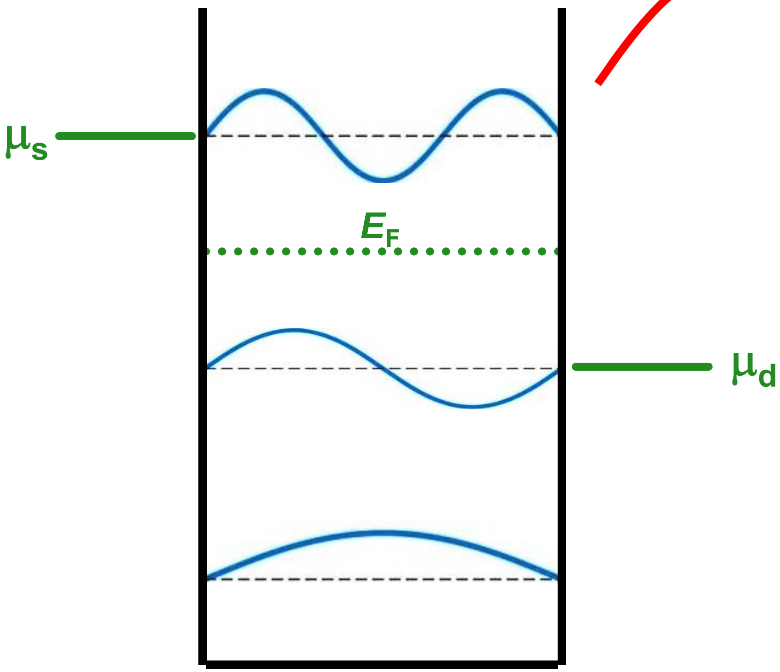


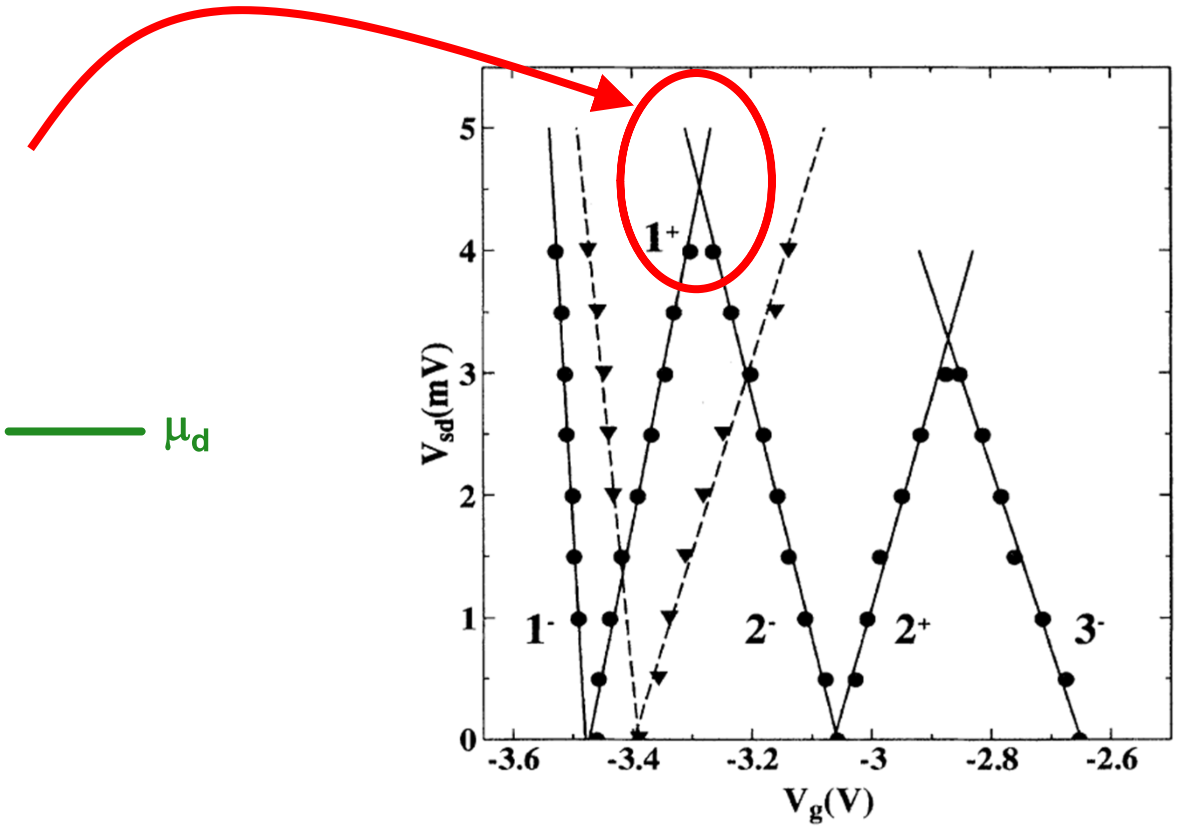


N.K. Patel *et al.*, PRB 44, 13549 (1991).



Measuring the 1D subband spacing

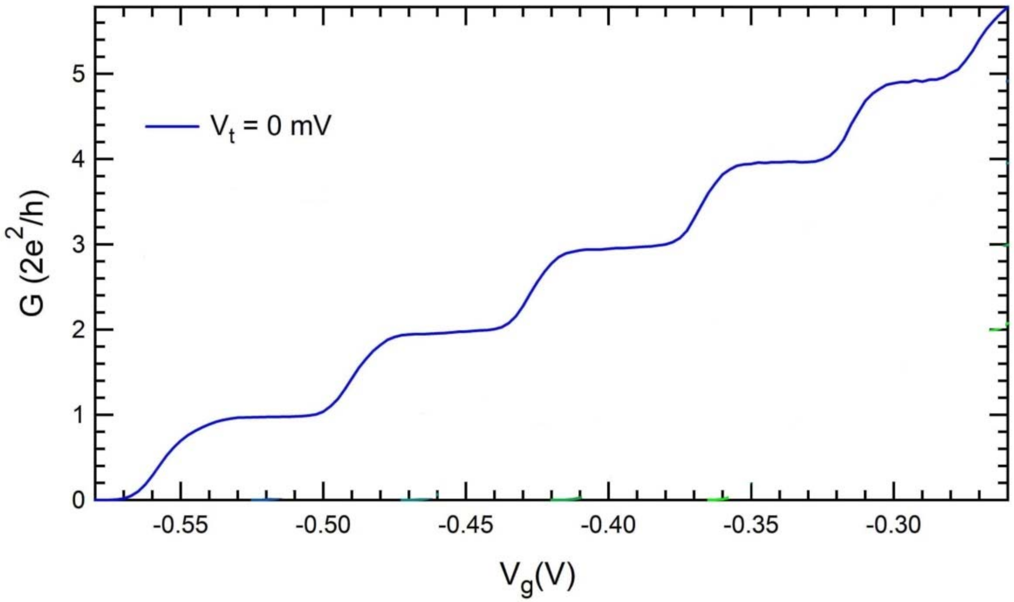


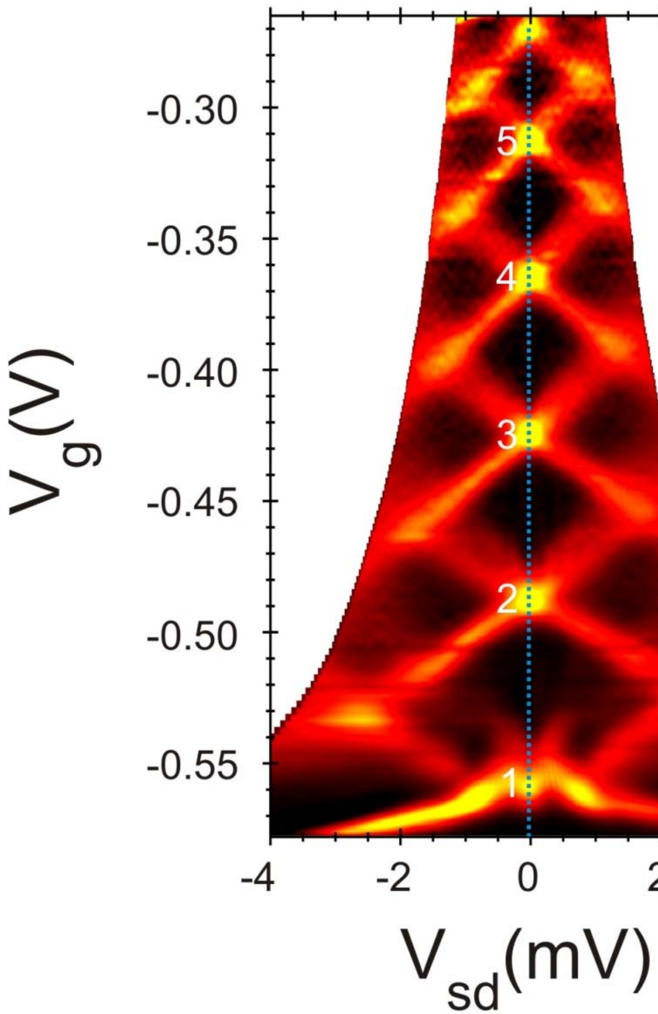


N.K. Patel *et al.*, PRB 44, 13549 (1991).

Measuring the 1D subband spacing

Now we plot the derivative of G vs V_g (called the transconductance) as a colour map against V_g and V_{sd}



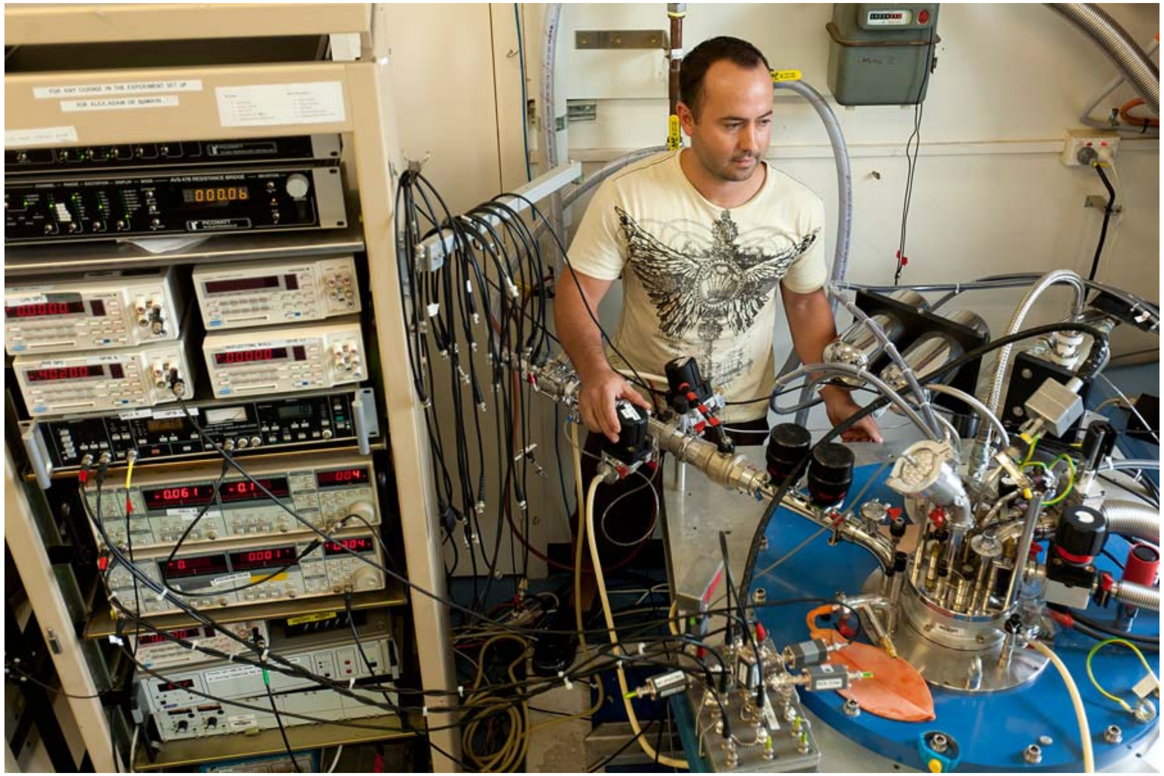


A.M. Burke *et al.*, Nano Lett. *in press*. doi: 10.1021/nl301566d

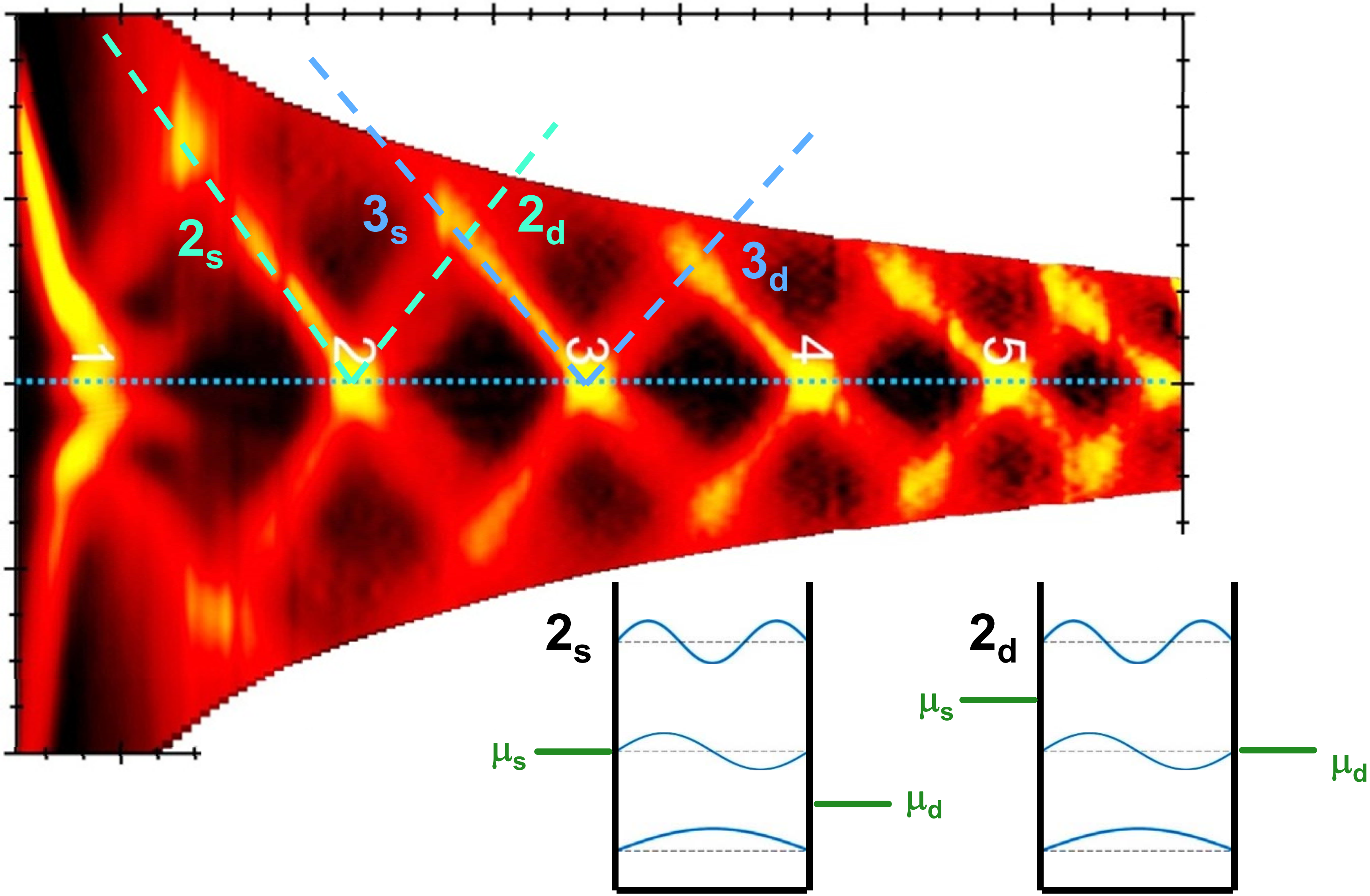
Experimental logistics

- **The typical 1D subband spacing for QPCs is of order 0.5 to 5 meV. To resolve the 1D subbands, one needs $k_B T \ll \Delta E$. This means $T \ll 5.5 – 55$K.**

- **Experiments are performed at low temperatures, typically below 4K, and as low as 50 mK.**

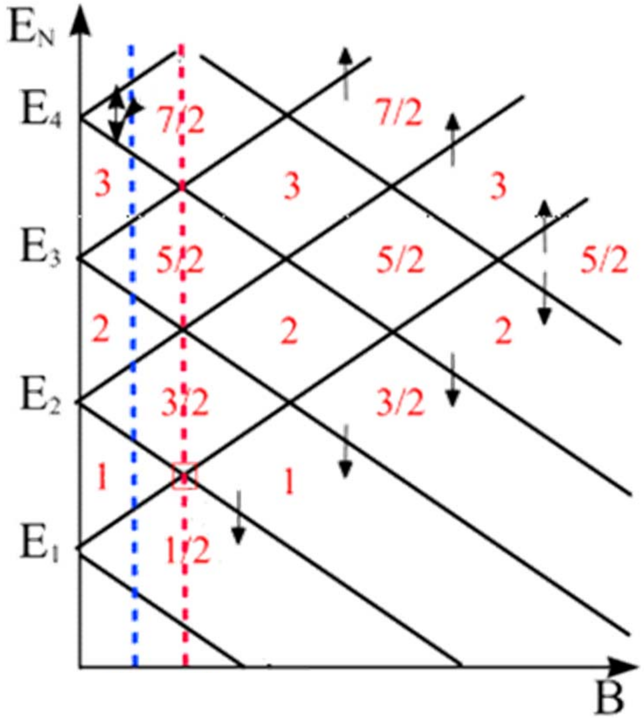


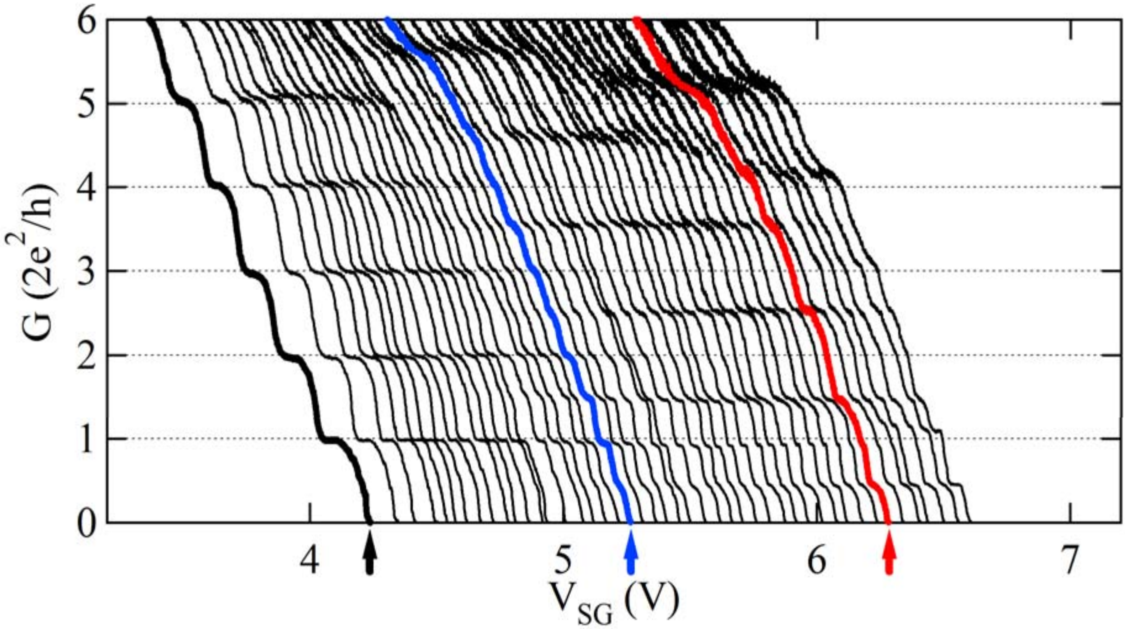
Tracking 1D subband edges



Breaking the spin degeneracy

- **At zero magnetic field, the 1D subbands are spin degenerate, hence the conductance steps of $2e^2/h$. As an in-plane magnetic field $B_{||}$ is applied, the 1D subbands will Zeeman split…**

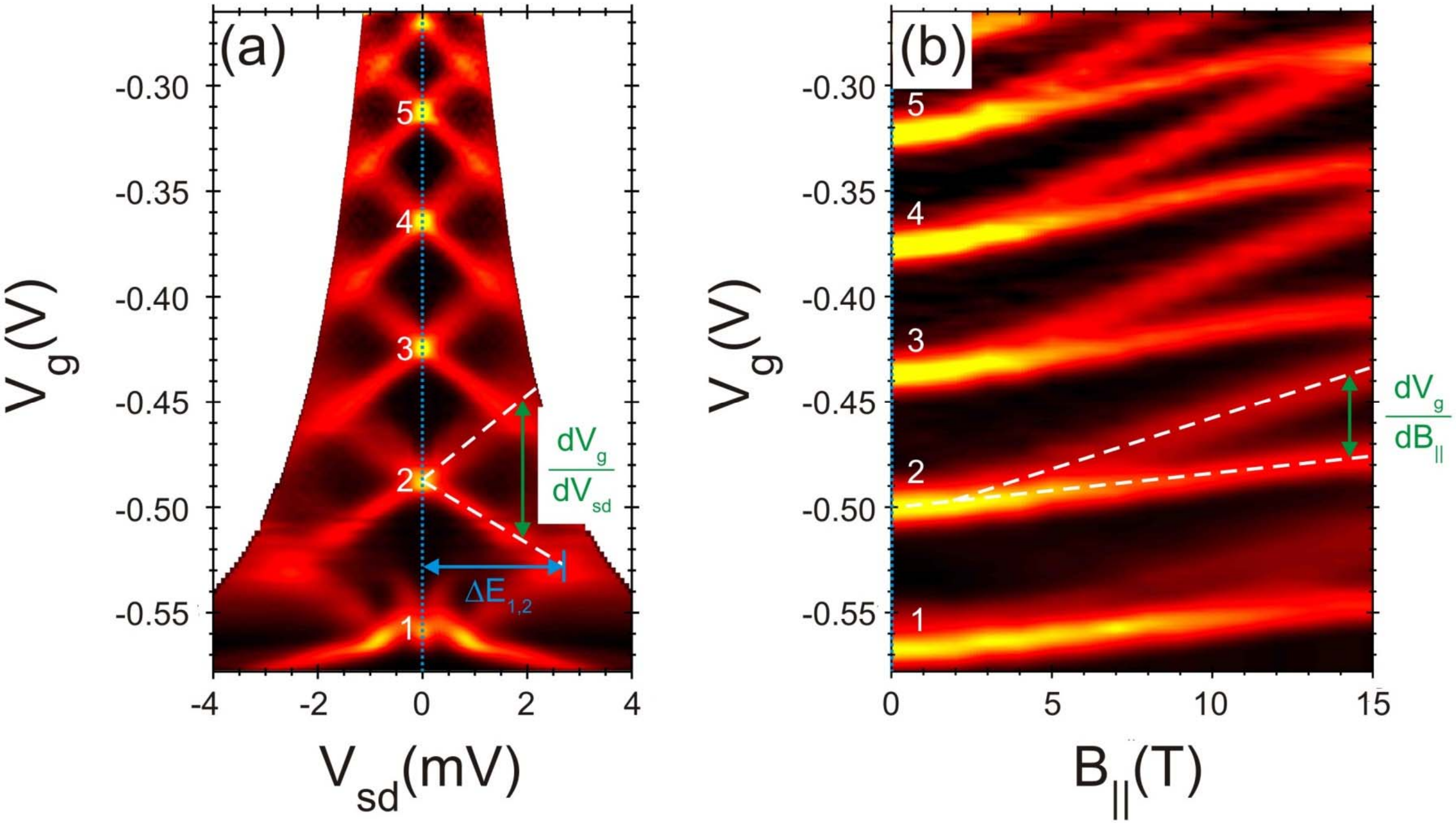




R. Danneau *et al.*, PRL 97, 026403 (2006).

Measuring the *g*-factor of the 1D subbands

$$\Delta E_z = e\left[\frac{dV_g}{dV_{sd}}\right]^{-1} \times \frac{dV_g}{dB_{||}} = e\frac{dV_{sd}}{dB_{||}} \longrightarrow g^* = \Delta E_z/\mu_B B_{||}$$

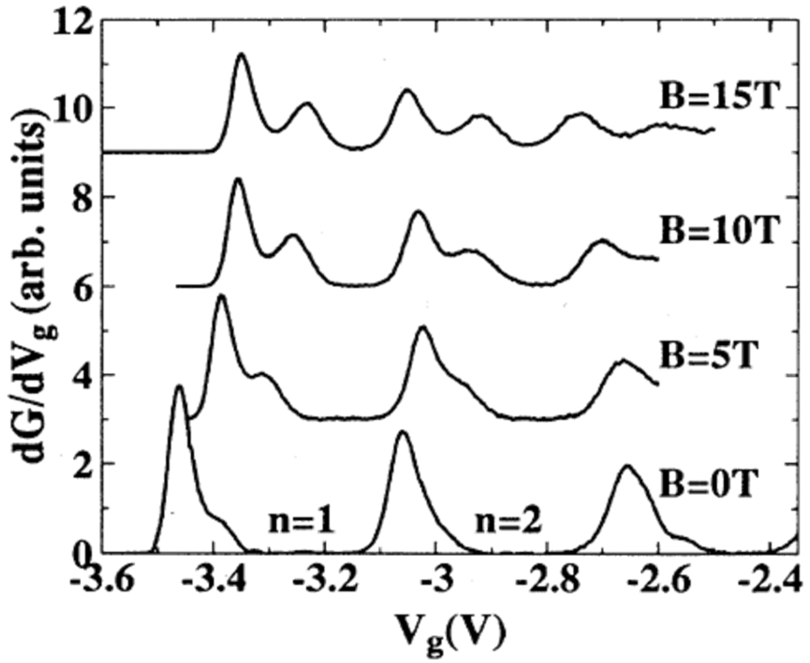


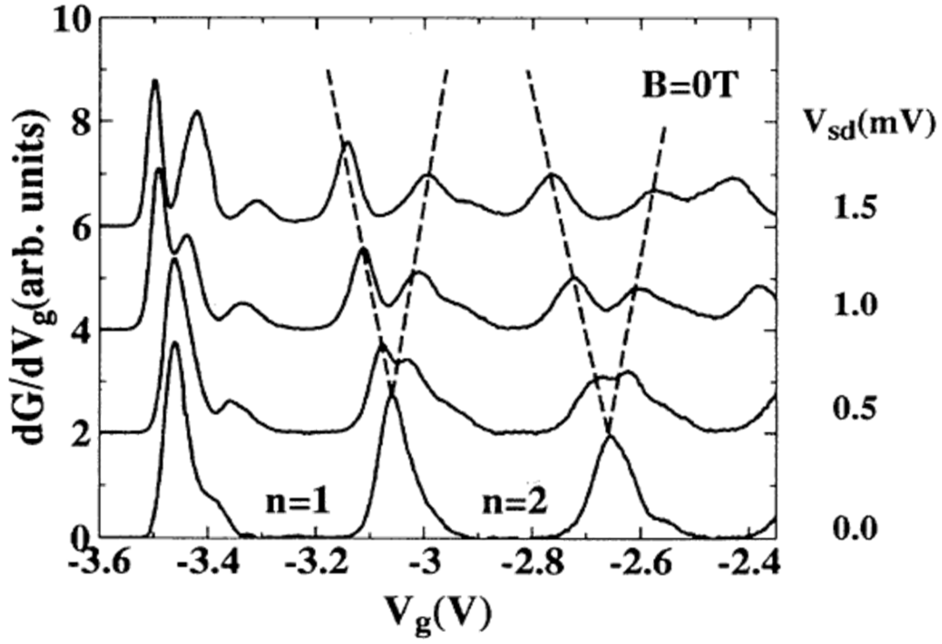
A.M. Burke *et al.,* Nano Lett. *in press*. doi: 10.1021/nl301566d

Measuring the *g*-factor of the 1D subbands

g^*_2 = 1.08

g^*_3 = 1.04

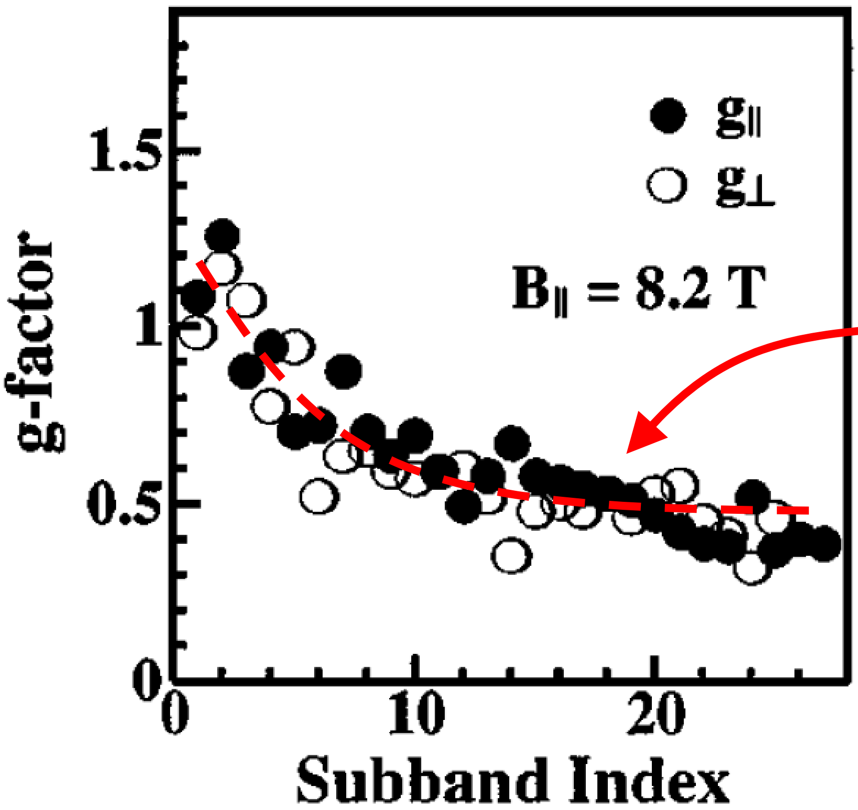




N.K. Patel *et al.*, PRB <u>44</u>, 10973 (1991).

*g** with 1D subband index

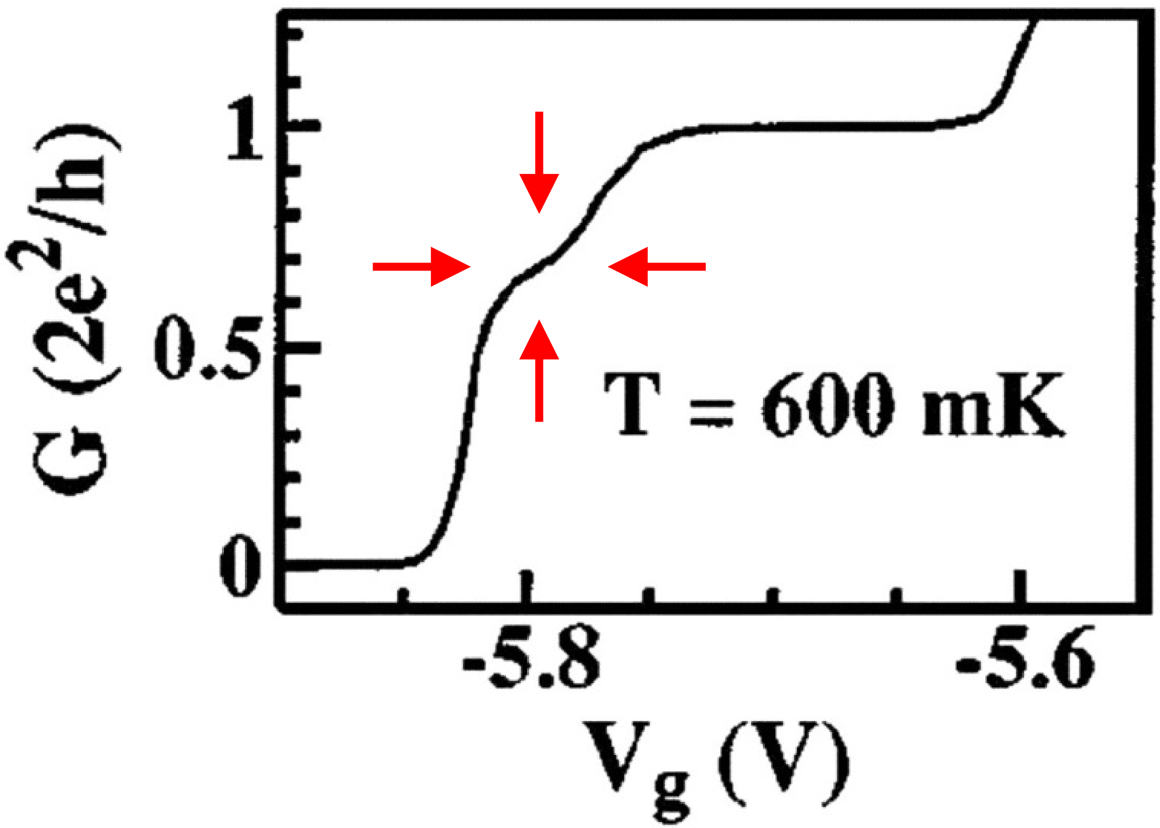
Rising *g as the channel is narrowed**
⇒ Exchange is important



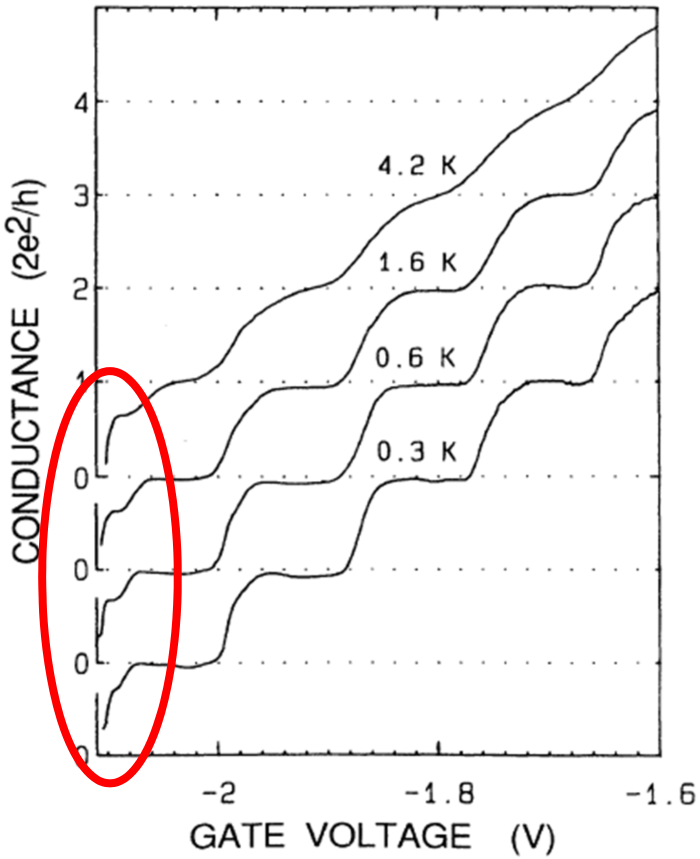
Exchange enhancement of g*

K.J. Thomas *et al.*, PRL 77, 135 (1996).

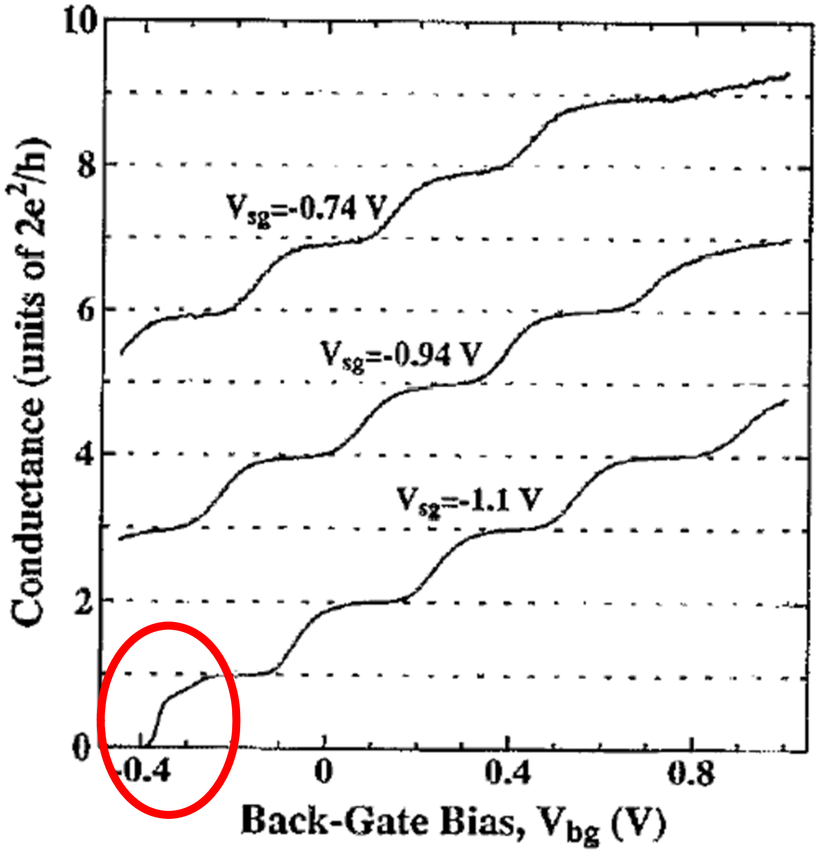
Time to introduce the 0.7 anomaly



The 0.7 anomaly has always been there



B.J. van Wees *et al.*, PRB 43, 12431 (1991).



A.R. Hamilton *et al.*, APL 60, 2782 (1992).

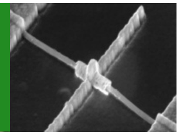
The first focused study was by Thomas *et al.*

VOLUME 77, NUMBER 1 PHYSICAL REVIEW LETTERS 1 JULY 1996

Possible Spin Polarization in a One-Dimensional Electron Gas

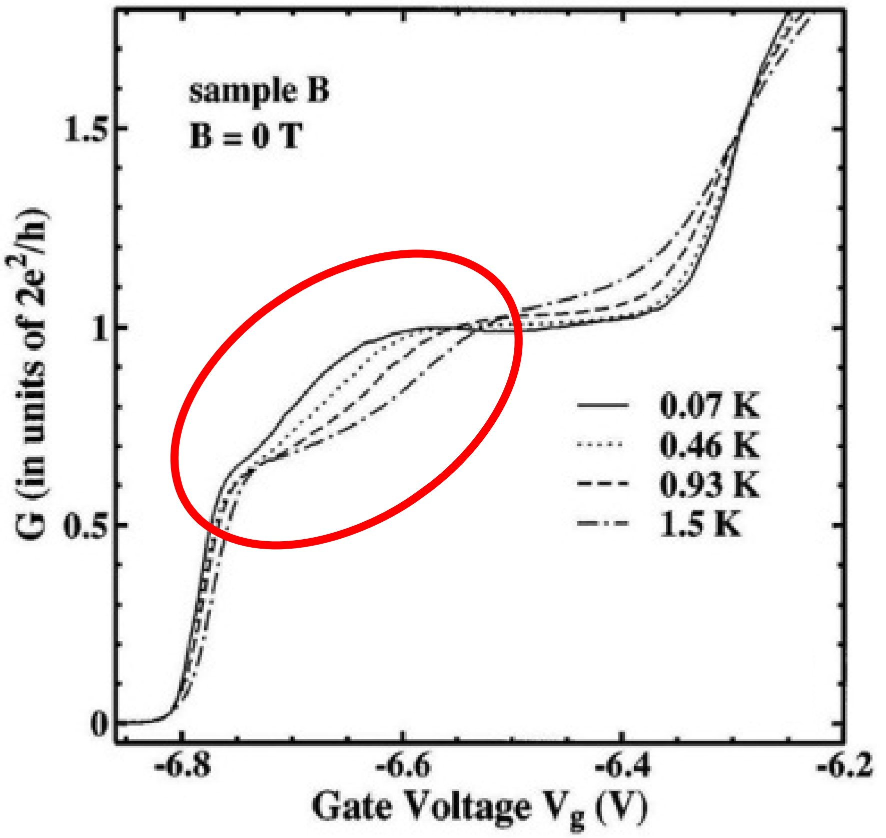
K. J. Thomas, J. T. Nicholls, M. Y. Simmons, M. Pepper, D. R. Mace, and D. A. Ritchie
Cavendish Laboratory, Madingley Road, Cambridge CB3 OHE, United Kingdom
(Received 4 March 1996)

In zero magnetic field, conductance measurements of clean one-dimensional (1D) constrictions defined in GaAs/AlGaAs heterostructures show up to 26 quantized ballistic plateaus, as well as a structure close to $0.7(2e^2/h)$. In an in-plane magnetic field all the 1D subbands show linear Zeeman splitting, and in the wide channel limit the g factor is $|g| = 0.4$, close to that of bulk GaAs. For the last subband, spin splitting originates from the structure at $0.7(2e^2/h)$, indicating spin polarization at $B = 0$. The measured enhancement of the g factor as the subbands are depopulated suggests that the "0.7 structure" is induced by electron-electron interactions. [S0031-9007(96)00520-0]



The temperature dependence of 0.7

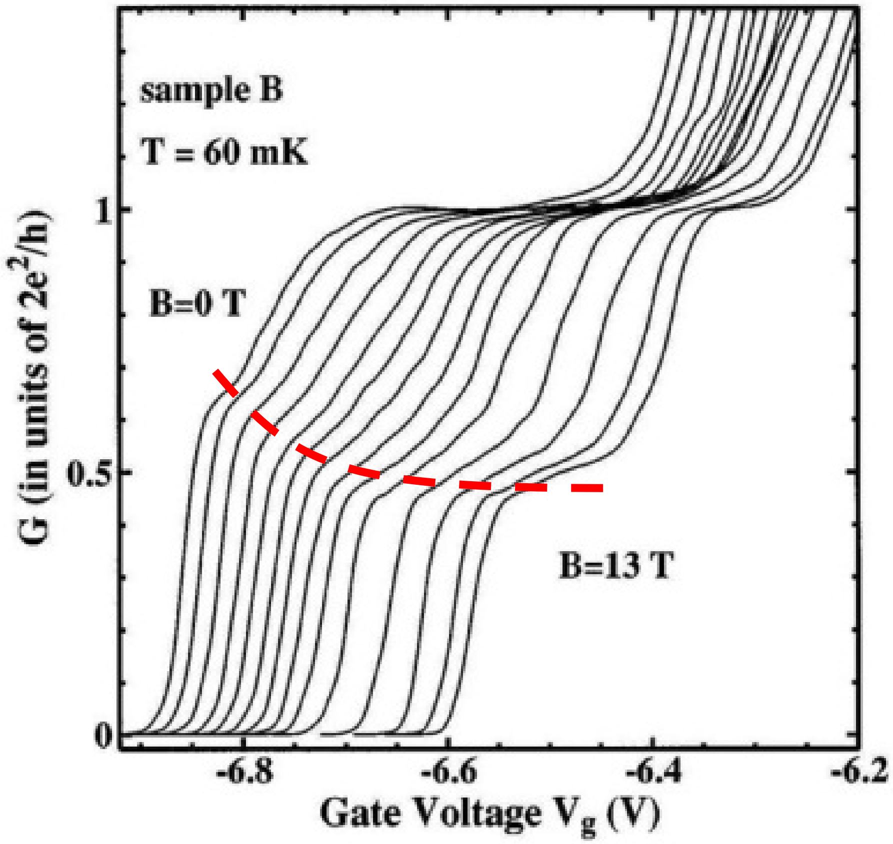
Strongest at intermediate temperature



K.J. Thomas *et al.*, PRL <u>77</u>, 135 (1996).

The in-plane field dependence of 0.7

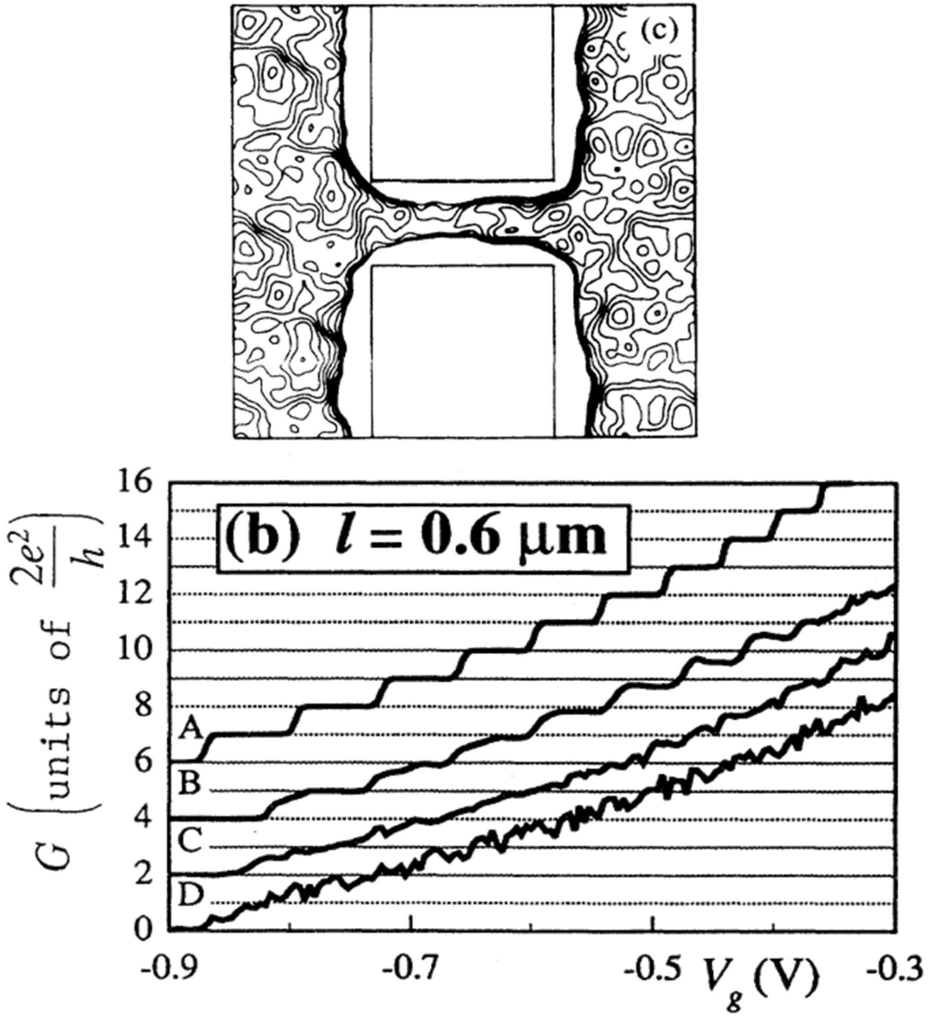
Drops to 0.5 with an in-plane magnetic field

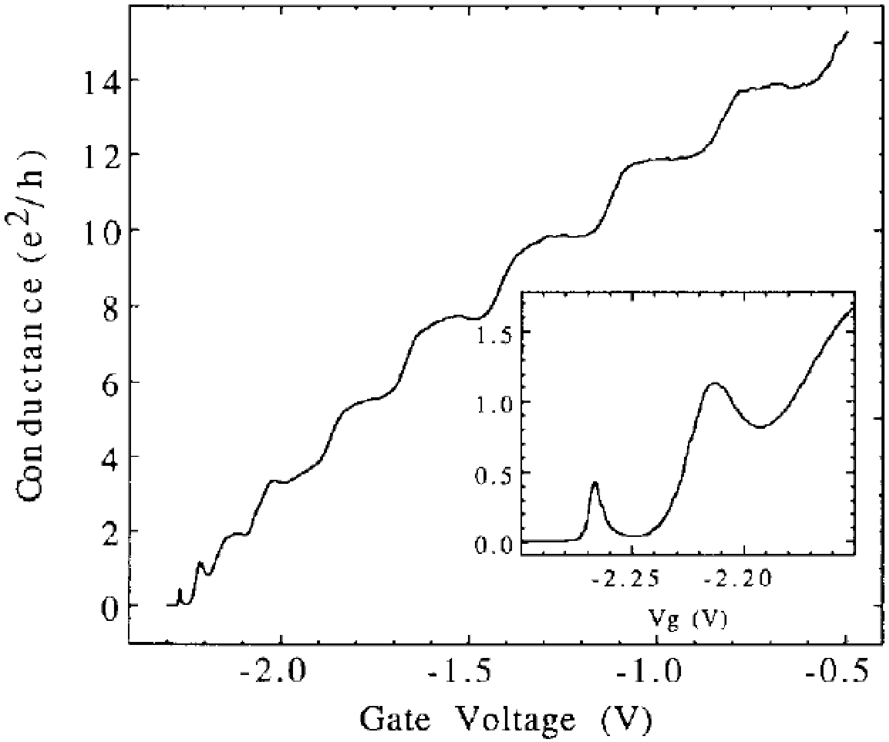


K.J. Thomas *et al.*, PRL 77, 135 (1996).

Is it just disorder?

We will return to this in Lecture 4





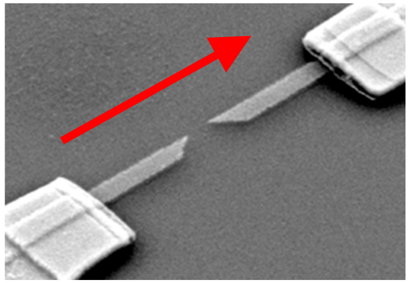
J.A. Nixon *et al.*, PRB 43, 12638 (1991).

P.L. McEuen *et al.*, Surf. Sci. 229, 312 (1990).

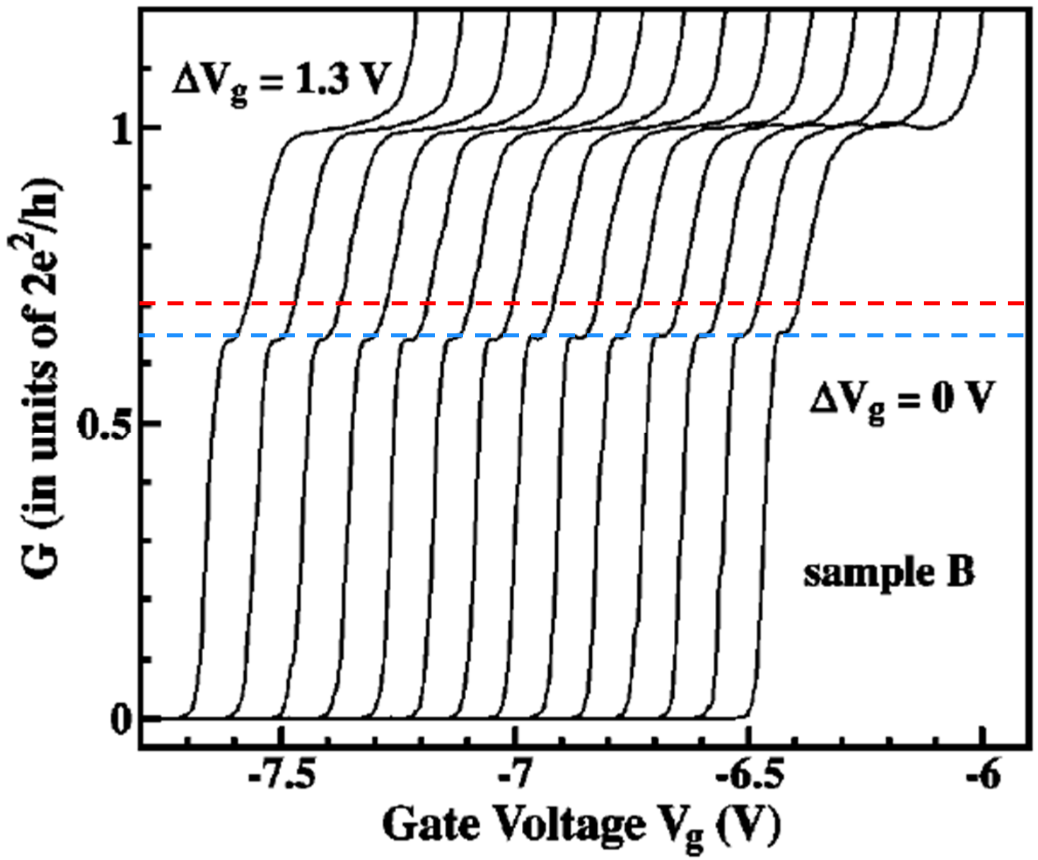
Channel shifting

Increasing ΔV_g moves the channel

$V_g + ½\Delta V_g$



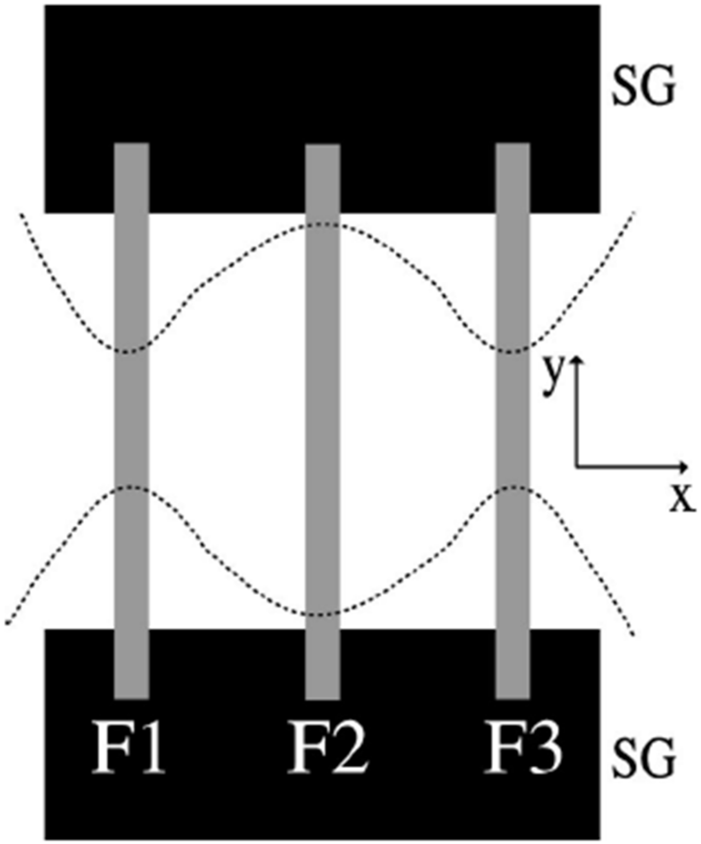
$V_g - ½\Delta V_g$

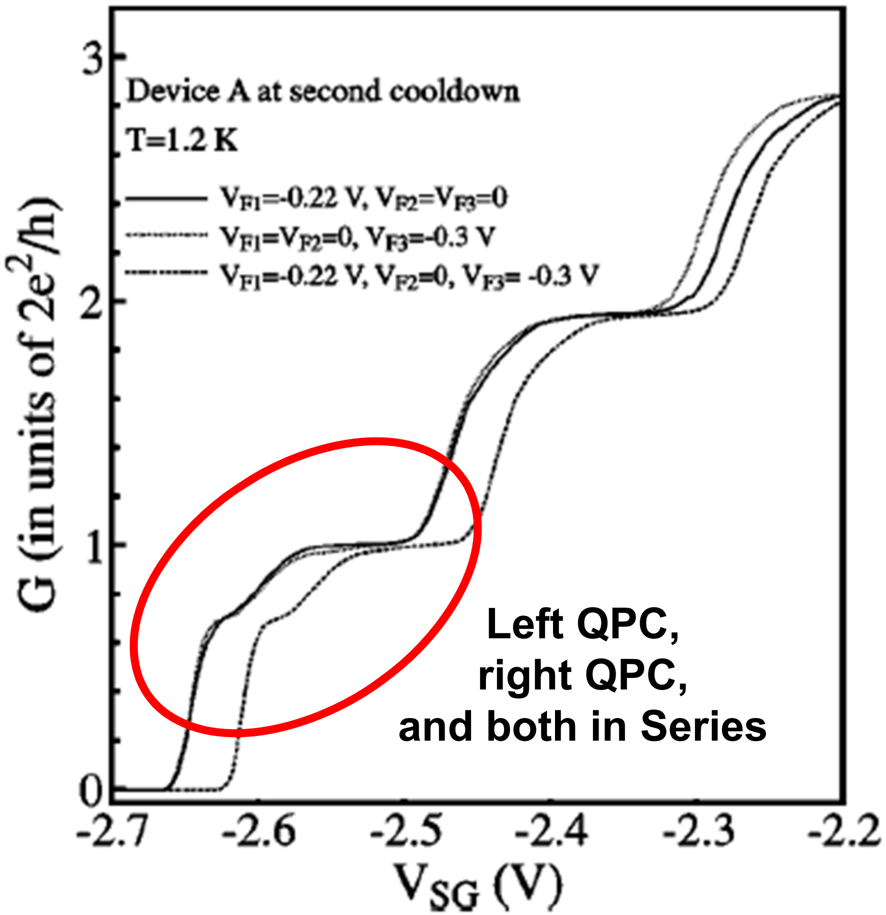


K.J. Thomas *et al.*, PRB 58, 4846 (1998).

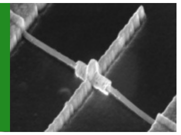
Further proof…

- **If 0.7 is a transmission resonance, it should be at 0.49 × 2*e*[2]/*h* for two QPCs in series.**





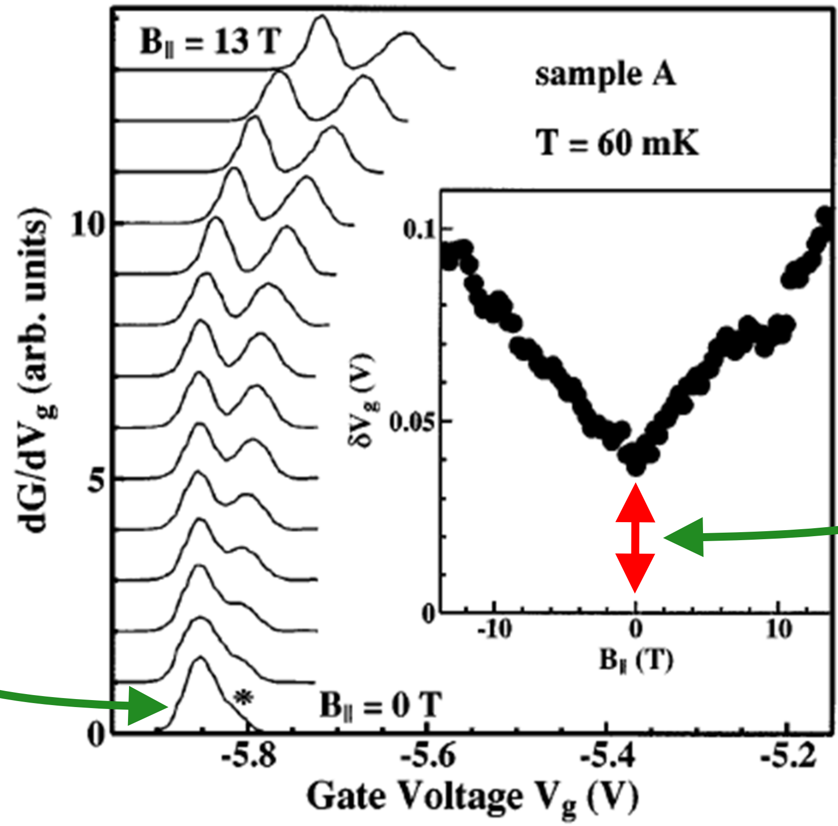
C.T. Liang *et al.*, PRB 60, 4846 (1998).



Initial hypothesis: Spontaneous spin polarization

- **The initial hypothesis proposed by Thomas *et al.* was that the 0.7 anomaly was due to spontaneous spin-polarization…**

If you look closely, it seems as though the spin-splitting doesn't go away at zero field.



Zero field spin-gap?

K.J. Thomas *et al.*, PRL 77, 135 (1996).

Initial theoretical support

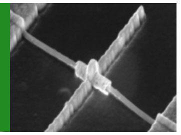
- **Set of two papers by Wang & Berggren using spin-density functional theory to investigate exchange and the possibility for zero-field spin polarization in 1D systems.**

- **First paper: Focus is on an infinite 1D system. The results reveal that the exchange interaction produces a large spin-splitting whenever the Fermi energy coincides with a 1D subband in energy. Full spin polarization predicted at sufficiently low electron density.**

C.K. Wang *et al.*, PRB 54, 14257 (1996).

- **Second paper: Focus is on a ballistic QPC potential in the lowest 1D subband limit. Spin-polarization occurs at the center of the QPC as density is lowered. This produces different effective barriers for spin-up and spin-down electrons.**

C.K. Wang *et al.*, PRB 57, 4552 (1998).



A primer on density functional theory

- DFT came about from a desire to extend beyond the Hartree-Fock (HF) model, and in particular, to include ‘correlation’ effects more accurately.

- ‘Correlation’ is basically the tendency for a many-body electron system to have non-homogeneities in density in order to minimize the overall energy of the system.

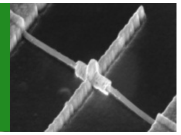
- Mathematically: Consider two electrons in a system, with $p(r_a,r_b)$ representing the probability density of finding one electron at r_a and one at r_b.

  The system is ‘uncorrelated’ if $p(r_a,r_b) = p(r_a)\mathrm{p}(r_b)$, and ‘correlated’ if the probability $p(r_a)$ depends on the position of electron b, and vice versa.

- There are essentially two types of correlation: Fermi and Coulomb.

  Fermi correlation: due to exchange, it prevents two electrons with parallel spins from occupying the same spatial location.

  Coulomb correlation: configures the charge in the system to minimize Coulomb energy, one example are Friedel oscillations, as charge reorders to screen charge.



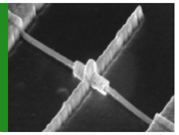
A primer on density functional theory

- **Fermi correlation is partially accounted for in HF theory. The antisymmetry requirement for the fermion wavefunction is built into the mathematical properties of the Slater determinant (the linear combination of Hartree products).**

$$\Psi(\mathbf{x}_1, \mathbf{x}_2) = \frac{1}{\sqrt{2}}\{\chi_1(\mathbf{x}_1)\chi_2(\mathbf{x}_2) - \chi_1(\mathbf{x}_2)\chi_2(\mathbf{x}_1)\}$$
$$= \frac{1}{\sqrt{2}}\begin{vmatrix}\chi_1(\mathbf{x}_1) & \chi_2(\mathbf{x}_1)\\ \chi_1(\mathbf{x}_2) & \chi_2(\mathbf{x}_2)\end{vmatrix}$$

It is partially accounted for because although electron exchange appears in the HF model, some aspects related to overall symmetry/spin of the system are not.

- **Coulomb correlation is not accounted for at all. This is the goal of methods like DFT. The difference between the calculated HF energy and the real energy is often called the correlation energy. This correlation energy is not all contributions from correlation though, because some are included in the HF model by the exchange term.**



A primer on density functional theory

- **The idea behind DFT stems from a theorem by Hohenberg and Kohn:**

  "There exists a universal function of the density $F[n(r)]$, independent of the external potential V(r), such that the expression $E \equiv \int V(r)n(r)dr + F[n(r)]$ has as its minimum value the correct ground state energy associated with $V(r)$."

  P. Hohenberg and W. Kohn, Phys. Rev. 136, B864 (1964).

- **$F[n(r)]$ is a functional = A function of a function.**

- **Kohn and Sham introduced a form that divides off the exchange and correlation contributions to the energy as a separate, individual term $E_{xc}[n(r)]$:**

$$E[n] = T_0[n] + \int d\mathbf{r}\, n(\mathbf{r})[V_{ext}(\mathbf{r}) + \tfrac{1}{2}\Phi(\mathbf{r})] + E_{xc}[n]$$

  where T_0 is the kinetic energy at density n if there are no electron-electron interactions, Φ is the classical Coulomb potential for electrons, and E_{xc} is the exchange – correlation energy.

  W. Kohn & L.J Sham, Phys. Rev. 140, A1133 (1965); R.O. Jones & O. Gunnarsson, RMP 61, 689 (1989).

Local density approximation

- There is no exact expression for $E_{xc}[n]$ for arbitrary n, and so various approximate expressions are required. The implementation of E_{xc} is where DFT gets hard. There are two very commonly used approximations:

- 1 – Local density approximation (LDA):

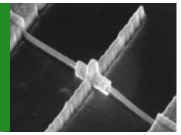
$$E_{xc}[n] = \int n(\mathbf{r})\,\epsilon_{xc}(n(\mathbf{r}))\,d\mathbf{r}$$

where ε_{xc} is the exchange and correlation energy per electron of a uniform electron gas of density n. The approximation works if $n(r)$ is sufficiently slowly varying, or alternatively, you can split off exchange to treat it exactly:

$$E_{xc}[n] = E_x[n] + \int n(\mathbf{r})\,\epsilon_c(n(\mathbf{r}))\,d\mathbf{r}$$

and keep ε_c as the correlation energy per electron. The latter is essentially just the Hartree-Fock method, with an approximate correction for correlation effects.

W. Kohn & L.J Sham, Phys. Rev. 140, A1133 (1965).



Local density approximation

- There is no exact expression for $E_{xc}[n]$ for arbitrary n, and so various approximate expressions are required. The implementation of E_{xc} is where DFT gets hard. There are two very commonly used approximations:

- **2 – Local spin density approximation (LSDA):**

$$E_{xc}^{LSD} = \int d\mathbf{r}\, n(\mathbf{r}) \varepsilon_{xc}[n_\uparrow(\mathbf{r}), n_\downarrow(\mathbf{r})]$$

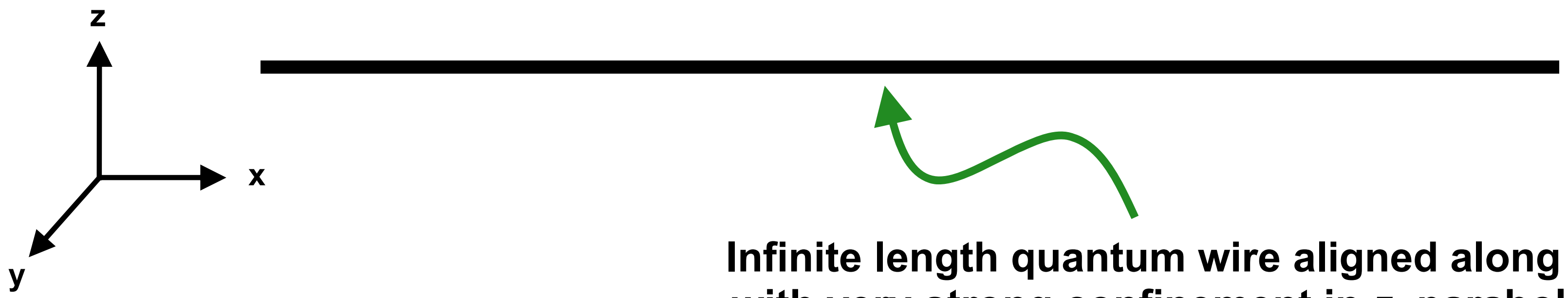
where $\varepsilon_{xc}[n_\uparrow, n_\downarrow]$ is the exchange and correlation energy per particle of homogeneous, spin-polarized electron gas with spin-up and spin-down densities $n_\uparrow(r)$ and $n_\downarrow(r)$, respectively.

- The LSDA allows more directly for variations in the spin-polarization, even at fixed electron density (i.e., $n(r)$ fixed with $n_\uparrow(r)$ and $n_\downarrow(r)$ changing).

R.O. Jones & O. Gunnarsson, RMP 61, 689 (1989).

DFT results for a 1D system

- In Wang's 1996 paper, the calculation is set up as follows:



Infinite length quantum wire aligned along *x*, with very strong confinement in *z*, parabolic confinement in *y* and a magnetic field *B* along *x*.

Start with a full Hamiltonian looking like:

$$\left(\frac{p_x^2 + p_y^2}{2m^*} + \frac{(p_z + eBy)^2}{2m^*} + V_{\mathrm{conf}}(y) + V_{\mathrm{conf}}(z) + V_H + V_{\mathrm{exch}}^{\sigma} + g\mu_B B\sigma \right) \psi^{\sigma}(x,y,z) = E^{\sigma} \psi^{\sigma}(x,y,z)$$

The confinement strength in *z* due to the heterojunction is much stronger than that in *y* due to the gates/etch defining the wire (level separation is ~100 meV vs ~1 meV). So we can use separation of variables:

$$\psi^{\sigma}(x,y,z) \simeq e^{ik_x x} \varphi^{\sigma}(y) \phi_1(z)$$

C.K. Wang *et al.*, PRB 54, 14257 (1996).

DFT results for a 1D system

and average over *z* to get:

$$-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial y^2}\varphi_l^\sigma(y)+[V_{\mathrm{conf}}(y)+V_H(y)+V_{\mathrm{exch}}^\sigma(y)+V_B(y)+g\mu_B B\sigma]\varphi_l^\sigma(y)=E_l^\sigma\varphi_l^\sigma(y)$$

This allows us to focus on the eigenfunctions in *y*, i.e., the 1D subbands. The five potentials in the Hamiltonian above are:

1: 1D confinement: $$V_{\mathrm{conf}}(y)=\tfrac{1}{2}m^*\omega^2y^2$$

2: Hartree potential: $$V_H(y)=-\frac{e^2}{4\pi\epsilon_0\epsilon}\int_{-\infty}^{\infty}n(y')dy'\{\ln[(y-y')^2]-\ln[(y_0-y')^2]\}$$

where: $$n(y')=\sum_\sigma n^\sigma(y')$$

and: $$n^\sigma(y')=\frac{1}{\pi}\sum_{E_l^\sigma\leq E_F}\left(\frac{2m^*}{\hbar}(E_F-E_l^\sigma)\right)^{1/2}|\varphi_l^\sigma(y')|^2$$

is the electron distribution for all occupied states with spin σ and $\varphi_l^\sigma(y')$ is normalized to 1.

DFT results for a 1D system

If we integrate the last expression over *y'*:

$$\sum_{\sigma} \sum_{E_l^\sigma \leq E_F} \left(\frac{2m^*}{\hbar}(E_F - E_l^\sigma) \right)^{1/2} = \pi n_{1d}$$

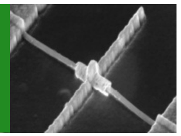
we get the 1D electron density n_{1D}, which is a specified constant in the calculations.

3: Exchange interaction: $$V^\sigma_{\text{exch}}(y) = -\frac{e^2}{\epsilon_0 \epsilon \pi^{3/2}} [n^\sigma(y)]^{1/2}$$

4: Magnetic field: $$V_B(y) = \frac{e^2 B^2 y^2}{2m^*}$$

5: Zeeman energy term: $g\mu_B B\sigma$

C.K. Wang *et al.*, PRB 54, 14257 (1996).

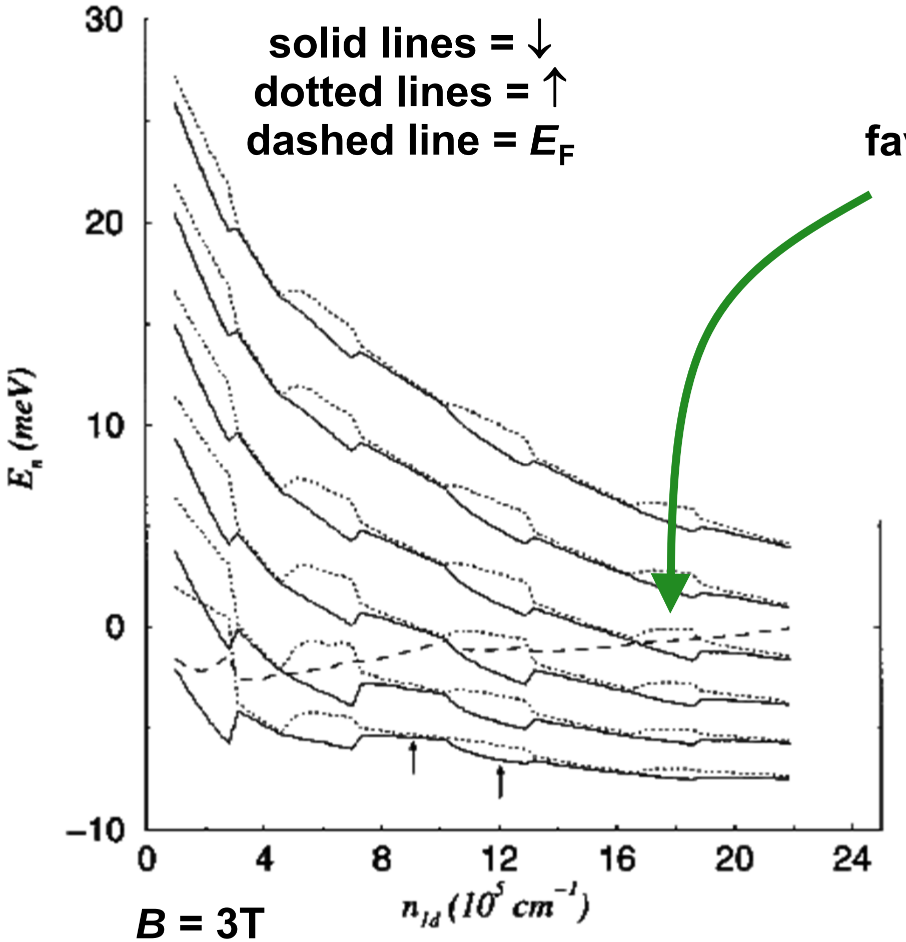


DFT results for a 1D system

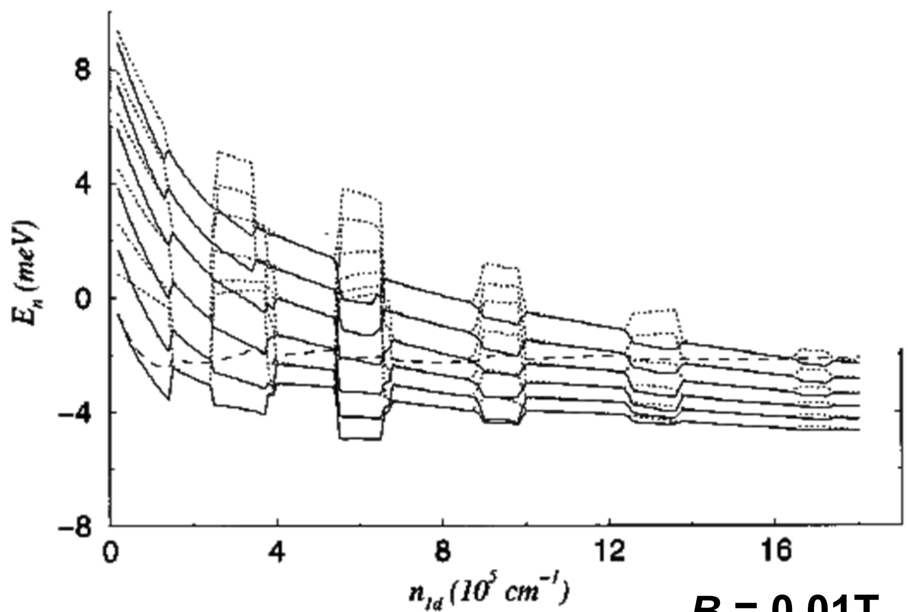
- **Solving the Kohn-Sham equations self-consistently as a function of n_{1D} gives:**

solid lines = ↓
dotted lines = ↑
dashed line = E_F

As a given 1D subband populates, the exchange interaction makes it more favourable to populate with ↓ electrons rather than ↑ electrons, until the subband fills.



***B* = 3T**

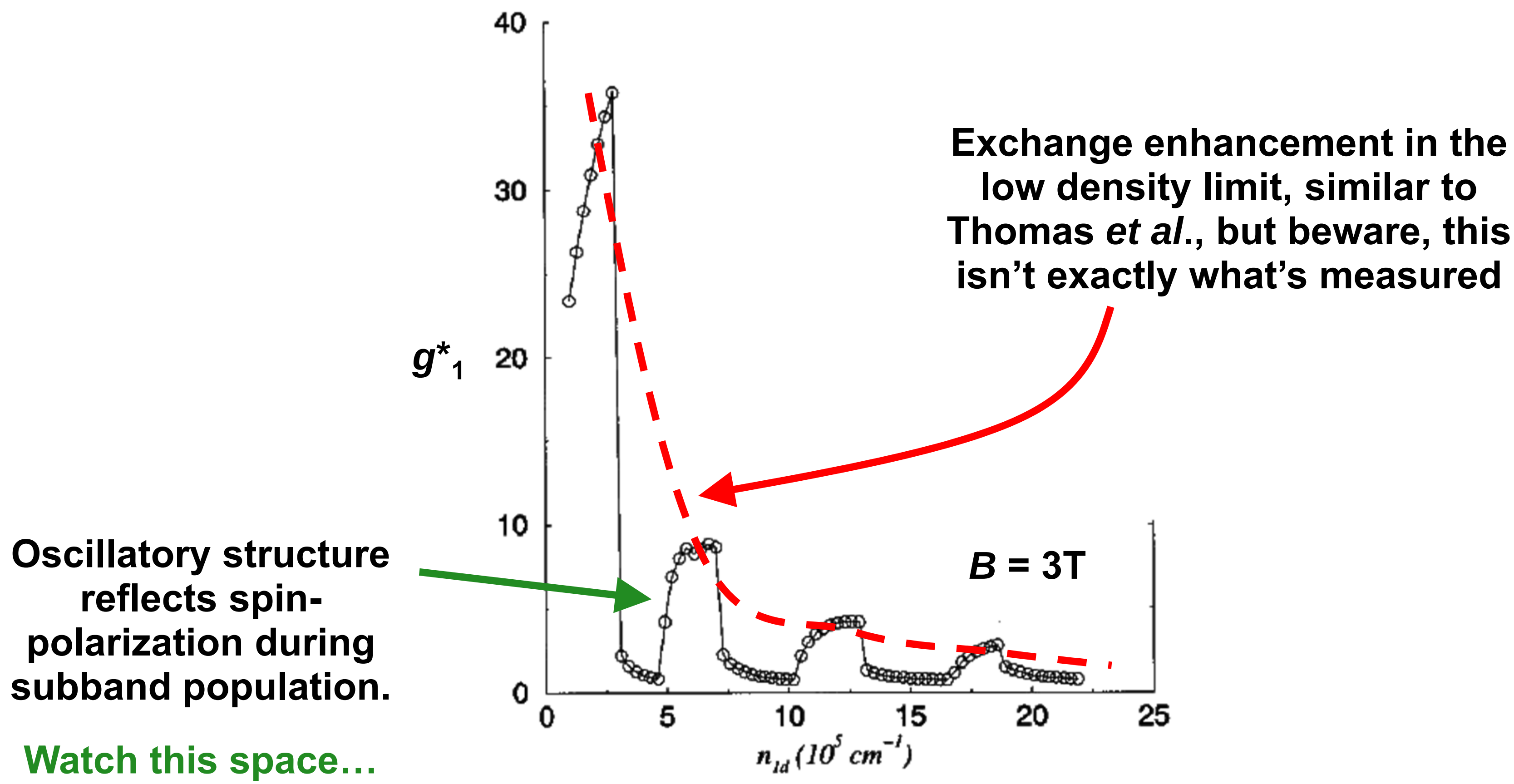


***B* = 0.01T**

C.K. Wang *et al.*, PRB 54, 14257 (1996).

DFT results for a 1D system

- **One outcome should be an oscillatory effective Lande *g*-factor *g** for each 1D subband. What's shown below is *g** for the 1st subband only. We will return to this…**

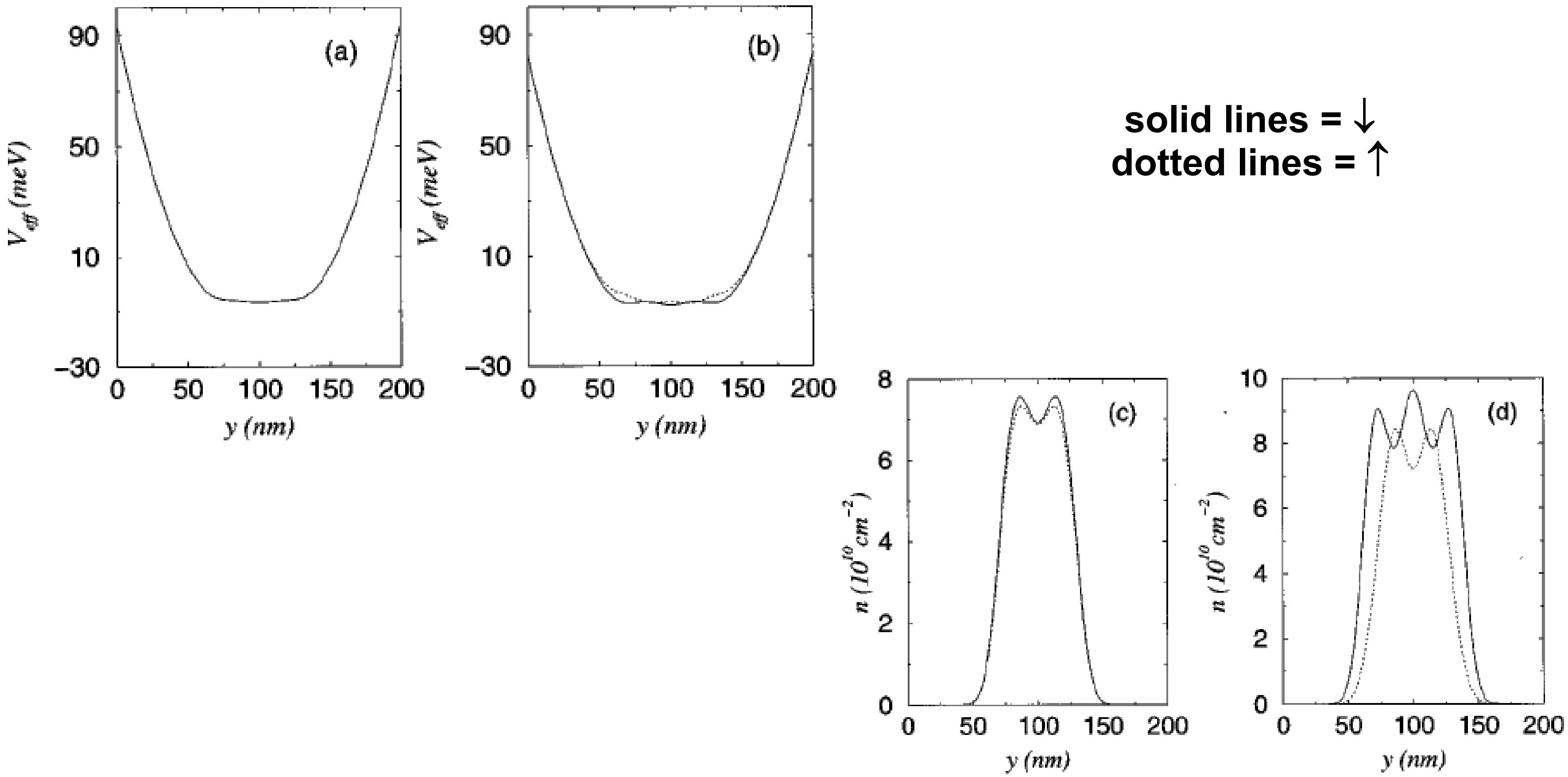


Watch this space…

C.K. Wang *et al.*, PRB 54, 14257 (1996).

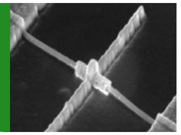
DFT results for a 1D system

- **Depending on n_{1D}, the effective potential for spin-up and spin-down electrons can be very similar or very different.**



solid lines = ↓
dotted lines = ↑

C.K. Wang *et al.*, PRB 54, 14257 (1996).



DFT results for a realistic QPC

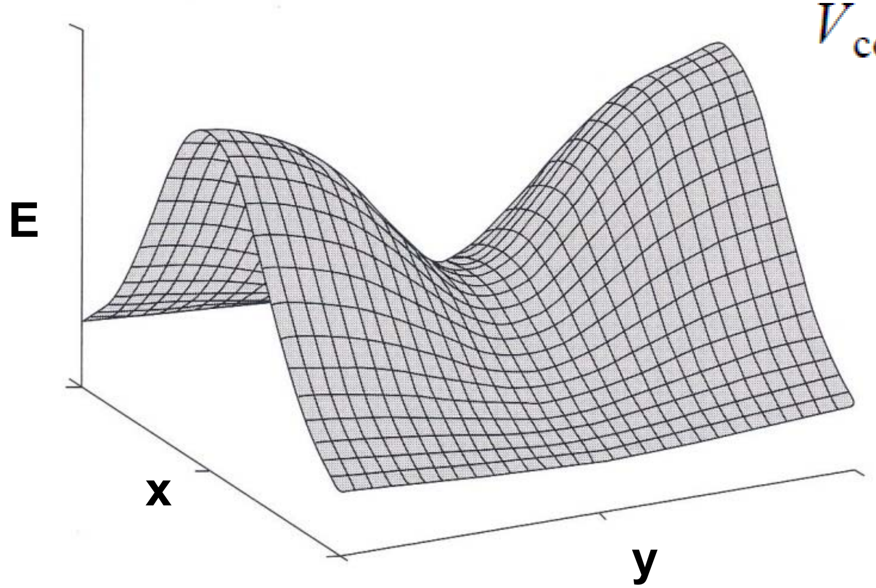
- **Wang's 1998 paper moves to a more realistic saddle-point potential for the QPC.**

$$V_{\rm conf}(x,y) = \frac{1}{2} m^* \omega_y^2 y^2 + \frac{V_0}{\cosh^2(\alpha x)}$$

in the small *x* limit, this reduces to:

$$V_{\rm conf}(x,y) \simeq \frac{1}{2} m^* \omega_y^2 y^2 - \frac{1}{2} m^* \omega_x^2 x^2 + V_0$$

with: $\omega_x = \sqrt{2\alpha V_0 / m^*}$



In the calculations $\hbar\omega_x$ = 1 meV and $\hbar\omega_y$ = 2 meV are used.

C.K. Wang *et al.*, PRB 57, 4552 (1998).

DFT results for a realistic QPC

- **Doing calculations with a 2D density/potential adds significantly to the computational cost, and this requires compromises in the model:**

  First, since the focus is 0.7, we can assume only the lowest 1D subband is occupied.

  Second, the Hartree term plays an insignificant role in the low density limit, and so this is dropped from the problem. The resulting Hamiltonian is:

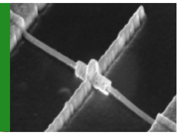
$$\left[\frac{p_x^2+p_y^2}{2m^*}+V_{\mathrm{conf}}(x,y)+V_{\mathrm{exch}}^{\sigma}(x,y)\right]\varphi^{\sigma}(x,y)=E^{\sigma}\varphi^{\sigma}(x,y)$$

- **The next step is to assume the potential is smooth in *x*, so that the adiabatic approximation can be used to write the wavefunction as:**

$$\varphi_{n,k}^{\sigma}(x,y)\simeq\Psi_n^{\sigma}(x,y)\Phi_k^{\sigma}(x)$$

Glazman & Jonson, JPCM 1, 5547 (1989).

C.K. Wang *et al.,* PRB 57, 4552 (1998).



DFT results for a realistic QPC

- **This allows the problem to be 'decoupled' as:**

$$-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial y^2}\Psi_n^\sigma(x,y)+[V_{\mathrm{conf}}(x,y)+V_{\mathrm{exch}}^\sigma(x,y)]\Psi_n^\sigma(x,y)=E_n^\sigma(x)\Psi_n^\sigma(x,y)$$

for the transverse motion with local energy $E_n^\sigma(x)$ and:

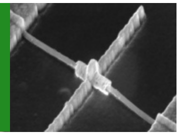
$$\frac{\partial^2}{\partial x^2}\Phi_k^\sigma(x)+(k^\sigma(x))^2\Phi_k^\sigma(x)=0$$

for the translational motion with local energy $E_k^\sigma(x)$.

- **The transverse energy $E_n^\sigma(x)$ acts as an effective, renormalized potential that the translational states $\Phi^\sigma(x)$ with energy $E_k^\sigma(x)$ have to penetrate.**

- **This gives the transmission through the QPC for a single electron with energy E^σ by solving the 2nd equation above once $E_n^\sigma(x)$ is known from the 1st equation above.**

C.K. Wang *et al.*, PRB 57, 4552 (1998).



DFT results for a realistic QPC

- **Practically, the exchange interaction requires a self-consistent approach accounting for all electrons in the lowest 1D subband.**

- **As in the pure 1D problem, the electron density is important. Integrating over $\Psi_1^\sigma(x,y)$ gives the 1D density:**

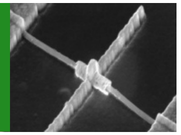
$$n_{1D}(x) = \sum_\sigma n_{1D}^\sigma(x) = \sum_\sigma \sum_k |\Phi_k^\sigma(x)|^2$$

with asymptotic limits:

$$n_{1D}(\pm\infty) = \sum_\sigma \frac{1}{\pi}\left(\frac{2m*}{\hbar}[E_F - E_1^\sigma(\pm\infty)]\right)^{1/2}$$

- **The Kohn-Sham equations are solved numerically, by first slicing the channel along x. The self-consistent solutions are found for each slice. For a given energy E^σ the electron distribution is solved, this is fed back with the constraint that $n_{1D}(\pm\infty)$ and the source/drain chemical potentials being held fixed, until E_F changes by less than 10^{-4} meV between iterations.**

C.K. Wang *et al.*, PRB 57, 4552 (1998).



DFT results for a realistic QPC

- **One last compromise is to take a semiclassical approximation for $n_{1D}(x)$:**

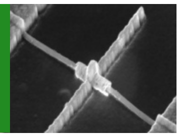
$$n_{1D}(x) = \sum_{\sigma} \left[\frac{k_F^{\sigma}}{\pi} + \frac{1}{4\pi(x_0 - x)} \left(1 - \exp^{-2q^{\sigma}(x_0 - x)}\right) + \frac{1}{4\pi(x_0 + x)} \left(1 - \exp^{-2q^{\sigma}(x_0 + x)}\right) \right]$$

with: $$k_F^{\sigma}(x) = \{2m^*/\hbar^2 [E_F - E_1^{\sigma}(x)]\}^{1/2}$$

and: $$q^{\sigma}(x) = [(2m^*/\hbar^2) E_1^{\sigma}(x)]^{1/2}$$

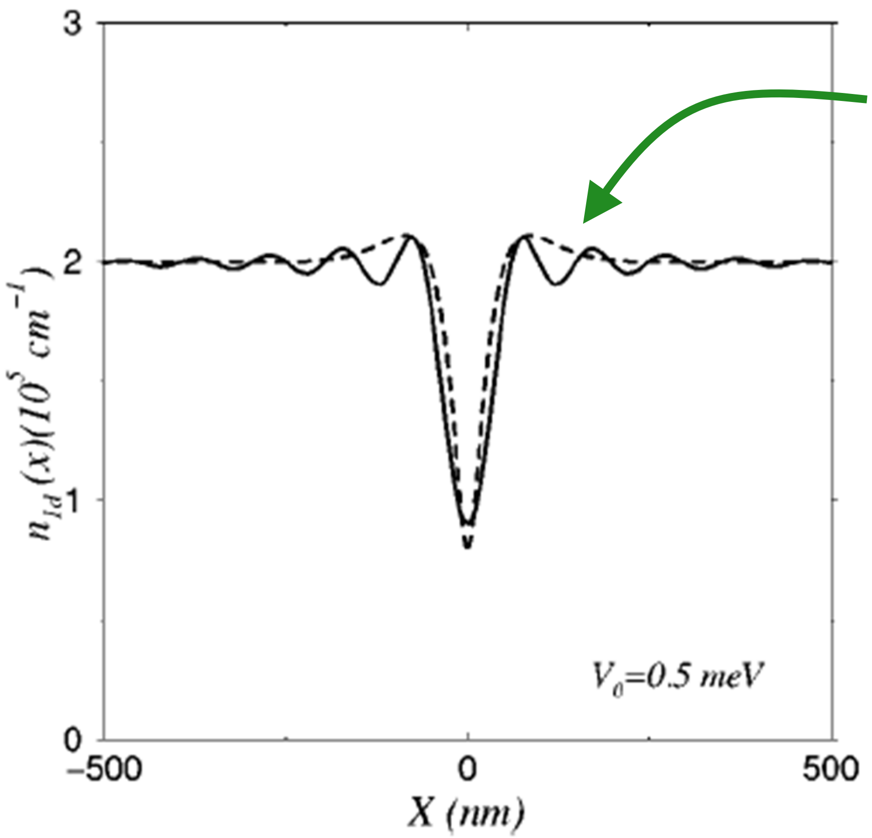
and where x_0 is the effective width of the barrier.

C.K. Wang *et al.*, PRB <u>57</u>, 4552 (1998).



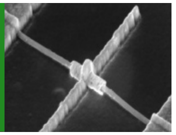
DFT results for a realistic QPC

- **The cost is the Friedel oscillations:**



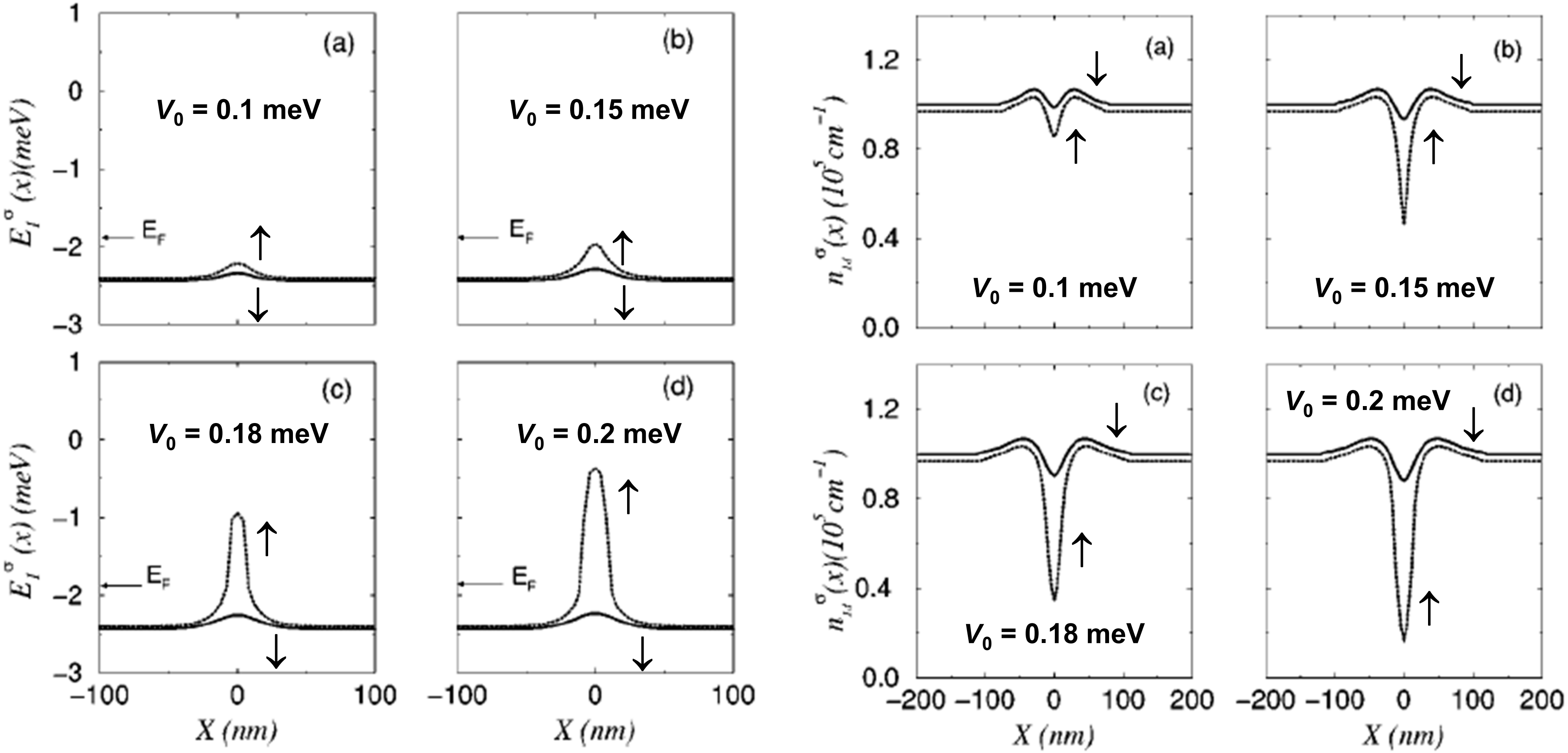
solid lines = exact
dotted lines = n_{1D} approx.

C.K. Wang *et al.*, PRB 57, 4552 (1998).



DFT results for a realistic QPC

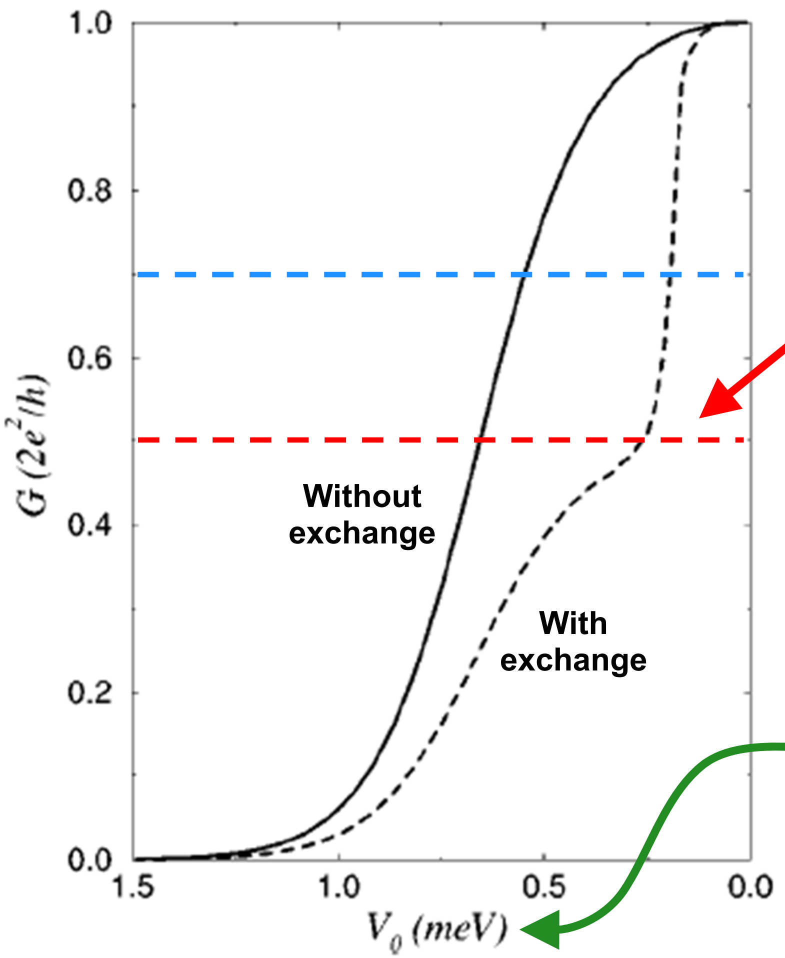
- The calculations show a barrier for spin up, relative to spin down at the centre of the QPC, and a corresponding spin polarization, accentuating with V_0.



All at $n_{1D} = 2 \times 10^5$ cm^{-1}

C.K. Wang *et al.*, PRB 57, 4552 (1998).

DFT prediction for the QPC conductance



Plateau at 0.5 not 0.7 but is clearly driven by exchange

Increasing V_o with fixed $\hbar\omega_x$ and $\hbar\omega_y$, roughly equivalent to pinching off the QPC.

C.K. Wang *et al.*, PRB 57, 4552 (1998).