Glazman Notes

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1 Main Take Away Points

The quantisation of conductivity in a 1D channel is relatively easy to derive using Landauer ideas. How sensitive is this idea of quantised conductance to adding in more realistic properties such as the length of the channel and the smoothness of the variation of confinement in the transverse direction?

For the quantised steps of conductance to exist we do not need a sharply bounded region with well-defined transversely quantised levels. It is the smoothness (adiabaticity) of the confining potential that is crucial. This was the unexpected result of the original QPC experiment, that it mimicked 1D behaviour despite it being more a point than a long wire!

Finally, this paper came out during the time when the argument of whether the conductance of a ballistic wire would be infinite or finite. The debate was because there would be no scattering and so Drude models predict an infinite acceleration from the applied electric field with no scatterings, but the Landauer approach predicted finite values with the resistance coming from the contacts. The difference in when these two models can be applied hadn't quite been discovered yet and it was the experimental QPC result that showed it was finite that really brought the Landauer formalism into the limelight.

1.1 Smaller Points and Examples

This paper uses quite simple mathematical tools of undergraduate quantum mechanics, to investigate something quite subtle. The focus is on the contacts (or accommodation regions) at the end points of the channel.

The second half when the dependence on the step shape requires some thinking about WKB approximations and Fermi functions and Landauer formulas. The transmission probability of a parabolic potential (the WKB stuff is just stated but derivation can be found elsewhere)

2 Notes on Paper

Previous estimates, put that the contact resistance was $\sim 2/e^2$ when the width of constriction was $\sim k_F^{-1}$ (ie the inverse quantum of conductance). Therefore this region has a considerable effect on the resistance and needs to be looked into. This is the debate hinted at earlier.

2.1 Set Up

We start with the width of the channel, $d(x)$ which will depend on the position x that it is at in the channel. Ignoring the curvature at the bottom of the well, which means to approximate the confining potential as a square well (which apparently matches experimental conditions, although I'm not quite sure how apart from the fact that there is a low density of electrons in QPC experiments so will all sit near the bottom of the potential) then the wavefunction, $\psi(x, y)$, can be written as the solution to the following equation:

$$-\frac{\hbar^2}{2m}\nabla^2\psi = E\psi, \qquad \psi(y = \pm d(x)/2) = 0 \tag{1}$$

where the wavefunction can be adiabatically separated so that $\psi(x, y) = \psi(x)\phi_x(y)$, where:

$$\phi_x(y) = \sqrt{\frac{2}{d(x)}}\ \sin(\pi n(2y + d(x))/d(x)) \tag{2}$$

as this is what obeys the boundary conditions and so the new equation we are dealing with is:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x) + \epsilon_n(x) = E\psi(x) + \frac{\hbar^2}{2m}\Big(2\frac{\mathrm{d}\psi_x(y)}{\mathrm{d}x}\frac{1}{\phi_x(y)}\frac{\mathrm{d}\phi_x(y)}{\mathrm{d}x} + \psi_x(y)\frac{1}{\phi_x(y)}\frac{\mathrm{d}^2\phi_x(y)}{\mathrm{d}x^2}\Big) \tag{3}$$
$$\text{where}\ \ \epsilon_n(x) = \pi^2 n^2\hbar^2/2md^2(x)$$

obtained from solving the equation for the quantised part (ie $\nabla^2\phi_x(y) = E\phi_x(y)$) to get the usual energy. Note that here in our analysis we have already assumed that there is smooth variation of $d(x)$ as we have adiabatically separated the wavefunction which assumes there is no component that scatters from the $\psi(x) \rightarrow \phi_x(y)$.

2.2 Lets Analyse

If the variation in $d(x)$ is smooth on the scale of k_F^{-1} (ie the electrons are basically a particle) then the effective potential $\epsilon_n(x)$ is semiclassical. This means the electron will see a smoothly varying potential and its like an early quantum mechanics problem! To be more specific, the variation of $\phi_x(y)$ with x will be slow enough that we can ignore all the derivative terms on the right hand side of the previous equation.

At larger n (which corresponds to higher energy states in the quantised direction), the effective potential will become so large that the total energy would become negative resulting a wavefunction that does not propagate (remember for a solution to propagate we need $-\nabla^2\phi = E\phi$ for positive ϕ otherwise the solution will be a decaying exponential. This marks the top of the accessible solutions in n below which all the quantised solutions in the y direction can propagate and above which they have a decaying exponential form. Tunnelling effects will be considered later.

Defining this top band as n_{max} and this point can be found from the fact that the momentum must be real for the mode to propagate, where the momentum is $p_n(X) = \sqrt{2m(E - \epsilon_n(x))}$. This must be real at the narrowest point which will be at $x = 0$ from the set up of the problem of gradually narrowing constriction that we have chosen to be symmetric about 0. Substituting in a form of the kinetic energy, $E = k^2\hbar^2/2m$ and setting $p_n(x) = 0$ gives the result:

$$n_{max} = [kd/\pi] \tag{4}$$

where the square brackets indicate the largest positive integer (floor function). States which have $n < n_{max}$, will contribute to the current and will have the following form

$$\psi_n(x) = \sqrt{\frac{p_n(\infty)}{p_n(x)}}\exp\Big\{\frac{i}{\hbar}\int_0^x p_n(x')dx'\Big\} \tag{5}$$

where this is simply an travelling wave that is normalised with a defined value of momentum. This comes from a WKB approximation.

2.3 So How Is This Conductance?

To find the conductance, the external electric field from the source-drain must be considered. As it will vary smoothly in the wire and have constant values $\pm E/2$ far in the reservoirs. It does not matter where we calculate the potential from (look at Datta chapter 2), so we chose to calculate it from a region of constant value of the potential. Remember that this is the differential conductance so $\frac{\mathrm{d}I}{\mathrm{d}V}\Big|_{V=0}$

Using Landauer ideas, the conductance is determined by the transmission matrix through coefficient matrix T_{nm} which correspond to the various channels. If it passes adiabatically through the constriction there is no mixing of the channels. This means the matrix has the form $T_{nm} = \delta_{nm}\Theta(n_{max} - n)$. Therefore the conductance is:

$$G = \frac{e^2}{\pi\hbar}\sum_n\sum_m T_{nm} = \frac{e^2}{\pi\hbar}\sum_n \Theta(n_{max} - n) = \frac{e^2}{\pi\hbar} n_{max}(k_F d) \tag{6}$$

2.4 What Does This Form Of Conductance Do?

So this will have sharp steps in the conductance at $k_F d = \pi n$, where k_F is the thing we vary, corresponding to varying the gate voltage in QPC experiments. Here this means when the fraction $k_F d/\pi$ hits the next integer number (or equivalently when k_F has increased by d/pi), the energy level above can be accessed and from the cancellation in the density of states and the velocity, this results in an extra quantum of conductance being allowed through. So to get the conductance from using Landauer, we did not even need to calculate the wavefunction form!

In the paper it is phrased like, a unit change in n_{max} is when the turning point/bottom of the band (ie. when $E = V$) passes through the centre of the constriction (ie $x = 0$) where $\epsilon_n(x)$ has a maximum. This essentially rephrases the above explanation, but up to now we have not considered quantum effects. The sharpness in the step is from the semiclassical approximation that we used, assuming the electron is a particle.

The corrections to this sharp step when at low temperatures are from tunnelling of modes that shouldn't propagate through and above barrier reflection of modes that should be able to - hence why the corrections are the same just below and just after the step. Keeping the adiabatic assumption ensures no mode mixing between the various quantised solutions.

The shape of the step, $\delta G((k_F d/\pi) - n)$, (so defined differently for each n) will depend on the curvature at the centre of the constriction, with radius of curvature R (so $\frac{\partial^2 d}{\partial x^2} = 2/R$). Here the notation for the shape of the step is a little confusing so to be explicit, the k_F is the variable we can control (the filling of our band) and δG has a specific form for each value of n. We must sum over n to get our total conductance, but the states where $n > n_{max}$ wont contribute and $n < n_{max}$ will contribute fully so the full conductance will simply be $G_n = n - 1 + \delta G$ with all the quantised solutions that can contribute fully as they are far enough from the current Fermi energy to have any significant quantum effects. The main quantum correction will be for $n \approx n_{max}$ with the calculation being what the transmission probability for a parabolic potential is.

Being further explicit, the form of Landauer that includes all the effects is

$$G = \frac{2e^2}{h}\int dE\ \left(-\frac{\partial f}{\partial E}\right)\mathrm{Tr}\big(\mathbf{t}\mathbf{t}^\dagger\big) \tag{7}$$

Here f is the Fermi function, and **t** is the off diagonal part of the $2n_{max} \times 2n_{max}$ scattering matrix. As we are still considering the adiabatic case, there is no mixing of channels and **t** will be a diagonal matrix, with each element giving the probability of transmission (via tunneling or above barrier reflection) for that specific channel energy. The Fermi energy allows for the higher energy modes to be populated by thermal fluctuations. Therefore there are two questions here, what are the effects from quantum tunnelling and what is the fluctuations due to temperature.

Therefore if we assume low temperature, then the derivative of the Fermi function becomes a step function, and we only have to sum over the transmission matrices. To obtain these transmission matrices, we first improve our definition of the potential to be x dependent rather than just the smallest part of the constriction. Calling $d(0) = D$

at the thinnest point (which means that $d'(x = 0) = 0$ as it is the thinnest point), we can expand the potential energy contribution,

$$\epsilon_n(x) = \frac{\hbar^2\pi^2 n^2}{2md^2(x)} \implies \epsilon''(x) = \frac{\hbar^2\pi^2 n^2}{2m}(\frac{6}{d^4}(d')^2 - \frac{2}{d^3}d'') \tag{8}$$

$$\epsilon_n(x) = \epsilon_n(0)\Big(1 - \frac{\partial^2 d}{\partial x^2}\Big|_{x=0}\frac{x^2}{D}\cdots\Big) \tag{9}$$

and then the equation we are trying to solve is:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}\psi_n(x)}{\mathrm{d}x} - \frac{2\epsilon_n(0)}{RD}x^2\psi_n(x) = (E - \epsilon_n(0))\psi_n(x) \tag{10}$$

and as we only care about solutions when E (which is the parameter we can change by altering the filling k_F as we are at zero temperature) we can set our measurement of energy to be around $\epsilon_n(0)$ by defining $E' = E - \epsilon_n(0)$ where we will drop the primed from now on. There are exact solutions to this sort of equation - parabolic cylindrical functions. So the plan is to now find the asymptotic solutions to the equation at $x \to \pm\infty$ and find the relation between the two asymptotic solutions which will give our transmission matrix and from Landauer our conductance!

So going to maths books we can find that for an equation:

$$-f''(z) - \frac{1}{4}z^2 f(z) = \mathcal{E}f \tag{11}$$

one pair of the asymptotic solutions in energy are:

$$F(\mathcal{E}, z \to \infty) \sim \frac{2}{y}\exp\bigg(i(\frac{y^2}{4} + \mathcal{E}\ln(y) + \frac{\phi}{2} + \frac{\pi}{4})\bigg) \tag{12}$$

$$F(\mathcal{E}, z \to -\infty) \sim i\frac{2}{|y|}\sqrt{1 + e^{-2\pi\mathcal{E}}}\exp\bigg(-i(\frac{y^2}{4} + \mathcal{E}\ln(y) + \frac{\phi}{2} + \frac{\pi}{4})\bigg) \tag{13}$$

$$- e^{-\pi\mathcal{E}}\exp\bigg(i(\frac{y^2}{4} + \mathcal{E}\ln(y) + \frac{\phi}{2} + \frac{\pi}{4})\bigg) \tag{14}$$

where ϕ here is related to the phase shift, which isnt important in the case we care about. But we need to be careful in finding out what parts are going in what direction. Each of these solutions is multiplied by $exp(i\mathcal{E}t)$ as we have dropped the time dependence from our equation we are solving. In the first term of the left hand side asymptotic we have a phase that will become more positive as y moves to the right with the time dependent part becoming more negative if we let time evolve forwards. So a point of phase will stay the same (ie propagate) if y increases and t increases if $\mathcal{E} > 0$ and so the first time is the incident wave.

Alternatively to identify which was is which, we can calculate the flux $j = -i(F^*F' - FF'^*$ which will be defined as satisfying the continuity equation.

From the asympototics and knowing which wave is the incident one we can relate the two $\psi_{in} = T\psi_{out}$ and then square the coefficient to get the probability of transmission for a given energy,

$$T = \frac{1}{1 + \exp(-2\pi\mathcal{E})} \tag{15}$$

where the modulus squared results in the phase shift part to not be relevant. As a quick note in many of the places online, they describe the asymptotic functions in terms of a gamma function and the following relation is crucial to relate the two,

$$\Gamma(\frac{1}{2} - i\mathcal{E}) = \sqrt{\frac{2\pi}{1+e^{-2\pi\mathcal{E}}}} e^{i\mathcal{E}} e^{i\phi} \tag{16}$$

So the final thing to do is to rescale our equation, into this reduced form to work out what $\mathcal{E}$ is. So by substituting in $x = lz$ and setting l to be such that the coefficient of the quadratic term vanishes we get

$$-\psi''(z) - \frac{4m\epsilon_n(0)l^4z^2}{\hbar^2 RD}\psi(z) = \frac{2mE}{\hbar^2}\psi(z) \tag{17}$$

$$-\psi''(z) - \frac{z^2}{4}\psi(z) = \frac{2mE}{\hbar^2}\sqrt{\frac{\hbar^2 RD}{16m\epsilon}}\psi(z) \tag{18}$$

$$\tag{19}$$

The final things we need to do is to only consider energies close to the maximum of a potential. This is done by completing the square on E,

$$E = \frac{\hbar^2}{2m}(k_F^2 - \frac{\pi^2 n^2}{D^2}) = \frac{\hbar^2}{2m}(k_F - \frac{\pi n}{D})(k_F + \frac{\pi n}{D}) \approx \frac{\hbar^2 \pi n}{2mD}(\frac{k_F D}{\pi} - n)(\frac{2\pi n}{D}) \tag{20}$$

So substituing in for this and for $\epsilon_n(0)$ we get that,

$$\mathcal{E} = \frac{2\pi^2 n}{4D^2}(\frac{k_F D}{\pi} - n)\sqrt{\frac{2RD^3}{\pi^2 n^2}} = \frac{\pi}{2}(\frac{k_F D}{\pi} - n)\sqrt{2R/D} \tag{21}$$

so substituting this into our general transmission result to get the quantum tunnelling effect on conductance as

$$\delta G(z) = \frac{2e^2}{h}\left[1 + \exp\left\{-z\pi^2\sqrt{2R/D}\right\}\right]^{-1}, \qquad z = (k_F D/\pi) - n \tag{22}$$

the overall result is from substituting $T_n = \frac{1}{1+\exp(-2\pi\mathcal{E}_n(R,D))} + \sum_n \Theta(n_{max} - n)$ into our Landauer formula to get a conductance in the form $G_0 + G_{tun}$.

This shows that the width of a step only weakly depends on the index. The numerical factor of $\pi^2\sqrt{2}$ also ensures that the steps are relatively sharp even for $R \sim d$. So we can formulate a condition for sharpness of steps: $\pi^2\sqrt{2R/D} > 1$

To show this conductance, there are two graphs at various values of R and D

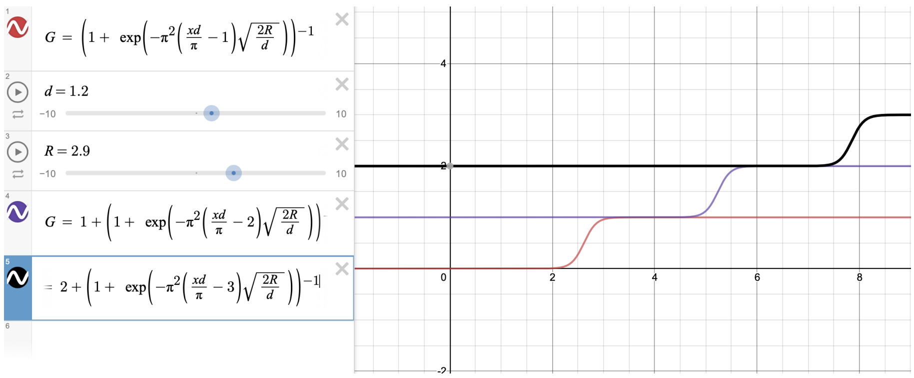

Figure 1: This is calculating the total conductance, where on the x axis we are varying the filling (k_F) through use of an external gate and the y axis is conductance. This clearly shows the discrete steps of the QPC experiment.

When temperature becomes relevant, we cannot assume that the derivative of the Fermi function is a step function anymore and that particles can be thermally excited above the step. So as we are dealing with fermions, this is

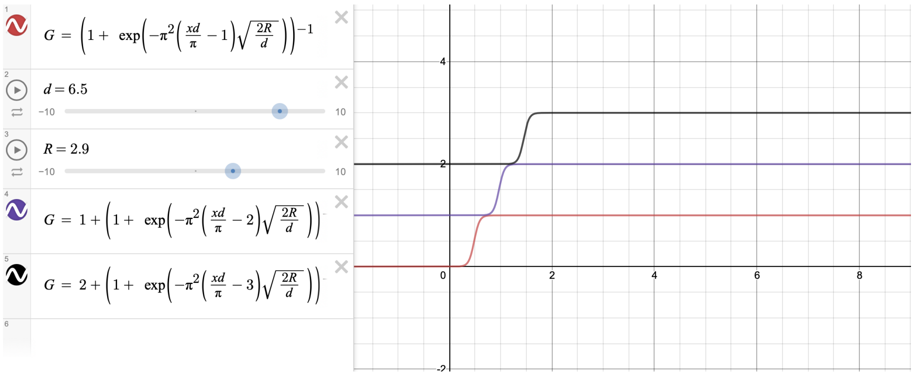

Figure 2: This is calculating the total conductance, where on the x axis we are varying the filling (k_F) through use of an external gate and the y axis is conductance. This as the width of the constriction is larger than the radius of curvature so we are approaching 2D behaviour and we can see the distance between the steps has decreased to a point where if the conductance sweep was performed (ie tracing along the highest line at any point) then we wouldnt be able to tell there was discrete steps.

modelled by the Fermi-Dirac distribution $(1 + \exp(-\beta(\epsilon - \mu)))^{-1}$. Remembering that the difference from the filling will be small to have the most chance of being excited we can use the same approximation that we did in E to get the result that (setting $k_B = 1$)

$$\delta G(z) = \frac{2e^2}{h}\left[1 + \exp\left\{-z\frac{\hbar^2\pi^2 n}{mD^2T}\right\}\right]^{-1} \tag{23}$$

and this form will be relevant when the temperature is enough to equal the contribution from tunnelling alone ie when

$$\frac{\hbar^2\pi^2 n}{mD^2T} \approx \pi^2\sqrt{2R/D} \implies T_{tun} = \frac{\hbar^2 n}{2mRD} \tag{24}$$

They obtain a slightly different formula in the paper though I imagine that this is from being slightly more specific with the above argument. If there is mixing between channels this will not completely destroy the quantisation of steps if there is a small chance of the channels being mixed - essentially what this means is that the general structure of the conductance as the sum over transmission matrices will (as its only a sum) be only slightly affected by channel mixing is the transmission matrix corresponding to it is small - a kinda circular statement!

Finally we can relate all of this to the length of the system by returning to our expansion of the potential and when it will continue to be accurate. As we only expand up to x^2/RD, we require that $L < \sqrt{RD}$. If it is larger than this then the electrons will be able to lose energy in these regions due to the width of the channel changing quickly enough and the voltage drop will be throughout the channel rather than at the contacts as is required for quantisation.

So we have found the length scale which all parameters must be larger than to ensure quantisation of conductance $\sqrt{RD}$ which shows that we dont need to fabricate long 1D wires to be able to test 1D phenomenon the smoothness of the constriction is the most important factor!

3 References

In these notes we used the Landauer formula without deriving it - so see any quantum transport book for this derivation. I prefer Datta's Electronic transport in Mesoscopic systems and Nazarov's Quantum Transport, but there is also good notes online from Quantum Transport Lecture Notes by Yuri M. Galperin (just put that in a search engine to find it)

The derivation of the exact transmission coefficient relies on properties of parabolic cyclindrical function with 'Quantum Mechanics of the Inverted Oscillator Potential' by Barton being my resource for this. There is also a cool WKB approximation to the reflection coefficient in the following notes

`http://web.mit.edu/8.322/Spring%202007/notes/reflectionabove030507.pdf`

Finally there is also reference to this in Quantum Effects near a Barrier Maximum - Ford, Hill et al in section 5.