PHYS-E055101 Low Temperature Physics: Nanoelectronics

Noise in electronic transport

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I. INTRODUCTION

Noise is an ubiquitous phenomenon in electronics, photonics, etc. The readings of a measuring apparatus will not in general be the same, but fluctuate around a mean value. Part of this comes from the imperfections of the measuring apparatus itself, and part from the device itself. These fluctuations will appear no matter how much we try to control the conditions of the experiment: ultimately, quantum mechanics will prevent us to obtain precise values of all possible observables due to the uncertainty relations. Another example is shot noise - to be discussed here - which is due to the randomness of electron or photon transfer. The effect of noise is typically detrimental to the functioning of a device, hiding the signal of interest. Therefore the noise needs to be quantitatively characterized, and parameters such as signal-to-noise ratio are of interest in almost any experiment. To reduce the noise, one option is to average over as many as possible individual readings, thus getting rid of the uncorrelated fluctuations. But the noise can also reveal information about new physics, and learning to extract this information is an additional experimental tool. In the much-quoted words of Rolf Landauer, "noise is the signal".

The field starts with the experiments done by Schottky in 1918, with electrons in vacuum tubes. Schottky realized that there are two types of noise in the vacuum tube, which he called *Wärmeeffekt* and *Schroteffect*. The first one is the thermal (Johnson-Nyquist) noise, the second became known as the shot noise. The shot noise for the completely uncorrelated particles is Poissonian, and it is reduced from this value by a number called Fano factor. Remarkably, as we will discuss, this suppression is in most cases not dependent on the parameters of the device, but only on the type of transport: for example, the Fano factor for the barrier junction is 1/2, for a chaotic cavity is 1/4, and for a disordered wire is 1/3.

II. BASIC PROBABILISTIC AND STATISTICS CONCEPTS

In this section we briefly review some elementary concepts from statistics. In typical mesoscopic problems, we are interested in the number N of electrons transferred trough a wire, junction, or device in a certain time Δt. This number N is in general random. Next, we define:

* the *average* of these random events: we repeat the experiment many times, sum the

number of events and divide by the number of repetitions to get the average $\langle N \rangle$.

* the *distribution* of the random events: we count how many times we get exactly N events and divide by the number of repetitions of the experiment, to get the probability P_N, normalized to 1, $\sum_N P_N = 1$.

For statistical independent events (say events of type A and events of type B) we can multiply the probabilities to find the probability of both occurrences: the probability of having N_A counts for the A event and N_B counts for the B event is thus

$$P_N^{(\text{A and B})} = P_{N_A}^{(A)} P_{N_B}^{(B)}. \tag{1}$$

As a result, the probability of having $N = N_A + N_B$ results is the convolution

$$P_N^{(\text{A or B})} = \sum_{N_A=0}^{N} P_{N_A}^{(A)} P_{N-N_A}^{(B)}. \tag{2}$$

Quiz: Prove that this probability is normalized, $\sum_N P_N^{(\text{A or B})} = 1$.

* the *moments* of the distribution are the averages of powers of N. The kth moment is

$$\langle N^k \rangle = \sum_N N^k P_N, \tag{3}$$

and of course the most used is the mean (average) $\langle N \rangle$

$$\langle N \rangle = \sum_N N P_N. \tag{4}$$

* the *characteristic function* of a probability distribution is

$$\Lambda(\chi) = \langle e^{i\chi N} \rangle = \sum_N P_N e^{i\chi N}. \tag{5}$$

The characteristic function is the generator of the moments of the distribution. Indeed, by expanding the exponential we get immediately

$$\Lambda(\chi) = \sum_{k=0}^{\infty} \frac{(i\chi)^k}{k!} \langle N^k \rangle, \tag{6}$$

or

$$\left. \frac{d^k \Lambda(\chi)}{d^k (i\chi)} \right|_{\chi=0} = \langle N^k \rangle. \tag{7}$$

* the kth order *cumulants* c_k of a distribution are defined thorough the natural logarithm of the characteristic function: the natural logarithm of the characteristic function is the generator of the cumulants of the distribution. This means that

$$\ln \Lambda(\chi) = \sum_{k=0}^{\infty} \frac{(i\chi)^k}{k!} c_k, \tag{8}$$

or

$$\left. \frac{d^k \ln \Lambda(\chi)}{d^k (i\chi)} \right|_{\chi=0} = c_k. \tag{9}$$

The second-order cumulant is the most used, and it is identical with the average of the fluctuation $\delta N = N - \langle N \rangle$ squared, (which is also called *variance*)

$$c_2 = \langle (\delta N)^2 \rangle = \sum_N N^2 P_N - \left(\sum_N N P_N \right)^2. \tag{10}$$

Higher-order cumulants are measured and calculated when one is interested in full counting statistics. The $k = 3$ cumulant is called *skewness* and the $k = 4$ cumulant is called *kurtosis*.

Exercise: By using a Taylor expansion for the logarithm, show that the second-order cumulant is indeed identical to $\langle (\delta N)^2 \rangle$ and that the skewness is the same as $\langle (\delta N)^3 \rangle$. Does this correspondence holds for $k \geq 4$?

A useful property of the characteristic function is

$$\ln \Lambda^{(\mathrm{A\ or\ B})}(\chi) = \ln \Lambda^{(\mathrm{A})}(\chi) + \ln \Lambda^{(\mathrm{B})}(\chi). \tag{11}$$

This result is very useful when we have two statistically independent types of events, because it allows to calculate the resultant characteristic function simply as a product $\Lambda^{(\mathrm{A\ or\ B})}(\chi) = \Lambda^{(\mathrm{A})}(\chi)\Lambda^{(\mathrm{B})}(\chi)$. It also allows us to prove the following: suppose we divide the time bin Δt over which we count the events into two time bins Δt_1 and Δt_2. Because the events in these two time bins are statistically independent, we have $\ln \Lambda(\chi, \Delta t) = \ln \Lambda(\chi, \Delta t_1) + \ln \Lambda(\chi, \Delta t_2)$. and $\Delta t = \Delta t_1 + \Delta t_2$. Now using Eq. (9) it follows that all the cumulants are directly proportional with the measurement time Δt. Of course, the more you measure, the larger the number of electrons that you will count as say hopping through a junction or the larger the number of decaying events that your counter will register: therefore it is natural that for example $\langle N \rangle$ increases. But the result above show that all the cumulants will grow linearly with the measurement time.

Examples

1] Uncorrelated transfer of electrons and the Poissonian distribution.

Consider now the case of uncorrelated transfer of electrons in one direction, with transfer rate Γ. This situation happens in tunnel junctions, where the transmission probabilities are small and therefore the electrons do not correlate with each other. In a small time interval dt the probability of transferring one electron is $P_1^{(dt)} = \Gamma dt$, and the probability of not transfer is $P_0^{(dt)} = (1 - \Gamma dt)$. Thus the characteristic function is

$$\Lambda_{dt}(\chi) = \langle e^{i\chi Q/e} \rangle = \sum_{n=0,1} P_n^{(dt)} e^{i\chi n} \tag{12}$$

$$= (1 - \Gamma dt) + (\Gamma dt) e^{i\chi} = \exp[\Gamma dt (e^{i\chi} - 1)]. \tag{13}$$

Now, as discussed above, since the electrons are uncorrelated, it follows that for a larger interval Δt we have

$$\Lambda_{\Delta t}(\chi) = \exp\left[\Gamma \Delta t (e^{i\chi} - 1)\right]. \tag{14}$$

To find now P_N corresponding to the interval Δt we take the inverse Fourier transform of the characteristic function,

$$P_N = \int_0^{2\pi} \frac{d\chi}{2\pi} \Lambda(\chi) e^{-iN\chi} = \tag{15}$$

$$= \int_0^{2\pi} \frac{d\chi}{2\pi} \exp[-iN\chi + \Gamma \Delta t (e^{i\chi} - 1)] \tag{16}$$

$$= e^{-\Gamma \Delta t} \int_0^{2\pi} \frac{d\chi}{2\pi} e^{-iN\chi} \sum_{n=0}^{\infty} \frac{1}{n!} (\Gamma \Delta t)^n e^{in\chi} \tag{17}$$

$$= \frac{(\Gamma \Delta t)^N}{N!} e^{-\Gamma \Delta t}. \tag{18}$$

This is called the *Poissonian distribution*. Note that to prove the last equality we used

$$\int_0^{2\pi} \frac{d\chi}{2\pi} e^{i\chi(n-N)} = \delta_{n,N}, \tag{19}$$

with $\delta_{n,N}$ the Kronecker symbol.

Similarly, you can convince yourself that by starting with the distribution Eq. (18) you obtain the correct characteristic function,

$$\Lambda_{\Delta t}(\chi) = \sum_{N=0}^{\infty} P_N e^{i\chi N} \tag{20}$$

$$= e^{-\Gamma\Delta t}\sum_{N=0}^{\infty}\frac{(\Gamma\Delta t e^{i\chi})^N}{N!} \tag{21}$$

$$= e^{(\Gamma\Delta t)[\exp(i\chi)-1]}. \tag{22}$$

The average number of transferred electrons can be found from this distribution and it is $\langle N\rangle = \Gamma\Delta t$. A property of the Poisson distribution is that the variance equals the mean, therefore $\langle N^2\rangle - \langle N\rangle^2 = \Gamma\Delta t$. Higher-order correlations can be calculated as well.

Poissonian current noise power. The current noise of Poissonian processes can be calculates easily. This is defined (see also next section, where we will do this more general and systematic) as double the fluctuations of the current $I = eN/(\Delta t)$,

$$S_{\rm P} = 2\langle(\delta I)^2\rangle = \langle\left(\frac{e\delta N}{\Delta t}\right)^2\rangle = 2\langle\left(\frac{eN}{\Delta t}\right)^2\rangle - 2\langle\left(\frac{eN}{\Delta t}\right)\rangle^2, \tag{23}$$

and now we know that the mean and variances of the number of electrons in an interval Δt are

$$\langle N\rangle = \Gamma\Delta t, \tag{24}$$

$$\langle(\delta N)^2\rangle = \Gamma\Delta t, \tag{25}$$

So the current and the shot noise is (see also Section 6.1.4. of [1] for an alternative detailed derivation)

$$\langle I\rangle = \frac{e}{\Delta t}\langle N\rangle = e\Gamma, \tag{26}$$

$$S_P = \frac{2e^2}{\Delta t}\langle(\delta N)^2\rangle = 2e^2\Gamma = 2e\langle I\rangle. \tag{27}$$

2. Transmission with zero fluctuations.

This happens in the case of ideal transmitting channels at zero temperature, where the wavefunction of the electrons is e^{ipz}, with well-defined momentum; thus the current is well-defined as well. The distribution in this case is $P_N = \delta(N - \bar{N})$ and the characteristic function is $\Lambda(\chi) = e^{i\chi\bar{N}}$.

III. TYPES OF NOISE

The central role in the definition of noise is played by the current-current correlation function

$$S_I(t,t') = 2\langle\delta I(t)\delta I(t')\rangle, \tag{28}$$

where $\delta I = I(t) - \langle I(t)\rangle$. This definition refers to classical currents, but it can be extended for the quantum case by considering the anticommutator $\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$ of the currents (which is symmetric in the current operators, therefore avoids the problem of noncommutativity of the current operator at different times),

$$S_I(t, t') = \langle\{\delta\hat{I}(t)\delta\hat{I}(t')\}\rangle, \tag{29}$$

and similarly $\delta\hat{I} = \hat{I}(t) - \langle\hat{I}(t)\rangle$. The quantity $S_I(t, t')$ is called *current noise power*, and similar quantities can be defined for the voltage and as combination of current and voltage. In stationary systems, S_I depends only on the difference in time $\tau = t' - t$, i.e. $S_I(t, t') = S_I(\tau)$. In this case, we can define the Fourier transform $S_I(\omega)$, called *noise power spectral density*,

$$S_I(\omega) = \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} S_I(\tau). \tag{30}$$

Fano factor: To characterize the noisiness of a system we need a benchmark: this benchmark is the Poissonian process discussed in the beginning. We will soon see that having sub- or above- Poissonian statistics is indicative of quantum effects. The quantity that makes this more precise is called the *Fano factor* F, defines as the ratio between S and the Poissonian noise S_P,

$$F = \frac{S_I}{S_P}. \tag{31}$$

So for every type of noise we can calculate this quantity.

The most usual types of current fluctuations encountered in mesoscopic physics and their noise power spectral densities are:

- *thermal noise:* (Nyquist-Johnson noise) : $S_I(\omega \approx 0) = \frac{4k_B T}{R}$, where R is resistance.
- *vacuum noise:* $S_I(\omega) = \frac{4\hbar\omega}{R}$, again for a resistance R.

  The thermal noise and the vacuum noise can be understood, in the case of linear systems in equilibrium, as resulting from the fluctuation-dissipation theorem. The proof is quite involved but can be found in many textbooks. The result is

$$S_I(\omega) = 2\hbar\omega Re[Y(\omega)] \left[\coth\left(\frac{\hbar\omega}{2k_B T}\right) + 1\right], \tag{32}$$

  where $Y(\omega)$ is the admittance of the sample.

Thermal noise is obtained when $\hbar|\omega| \ll k_B T$, in other words the system is at a high temperature (compared to the frequency). In this case, from Eq. (32) we get

$$S_I(|\omega| \ll k_B T/\hbar) = 4k_B T Re[Y(\omega)]. \tag{33}$$

If the impedance is a resistor, we get $S_I = 4k_{\rm B}T/R$. Vacuum noise is obtained when the temperature is small $k_B T \ll \hbar\omega$. In this case we the noise does not depend on temperature,

$$S_I(\omega \gg k_B T/\hbar) = 4\hbar\omega Re[Y(\omega)]. \tag{34}$$

- *shot noise:* $S_I(\omega \approx 0) = 2eFI$ where F is the Fano factor.

- *1/f noise:* this is a flicker noise due to coupling of the device to two-level fluctuators, impurities, or other unknown sources of fluctuation. 1/f noise means that the power spectrum decreases as a function of frequency, which in practice means that this source of noise is important at low frequencies, typically below 10 kHz. This source of noise is important in many devices, including circuits that aim at realizing a quantum processor, where it turns out to be an important source of perturbation. To some extend, this type of noise can be eliminated if the measurement is done fast enough. Although 1/f noise is an important topic, we will not discuss it further in this lecture, since it requires its own set of theoretical tools.

To understand in a rather general way why noise measurements can provide an important diagnosis tool for the physics, consider the classical (Boltzmann) versus the quantum statistics (Fermi and Bose-Einstein distributions) for systems at equilibrium in the form

$$\langle N\rangle = \frac{1}{e^{(E-\mu)/k_{\rm B}T} + x}, \text{ with } x = \begin{cases} 0 & \text{classical particles,} \\ -1 & \text{bosons,} \\ 1 & \text{fermions.} \end{cases} \tag{35}$$

Using this statistics one gets the fluctuation in the form

$$\langle(\delta N)^2\rangle = \langle N\rangle(1 - x\langle N\rangle). \tag{36}$$

Quiz: Prove this result. Hint: in the grand canonical ensemble, $\langle(\delta N)^2\rangle = k_{\rm B}T(d\langle N\rangle/d\mu)|_{V,T}$.

The classical case corresponds to $x = 0$ and we get the Poissonian result for the fluctuation, $\langle(\delta N)^2\rangle = \langle N\rangle$. In the case of quantum statistics, we have $\langle(\delta N)^2\rangle > \langle N\rangle$ for bosons,

a situation called *super-Poissonian* or *bunching*. With fermions, we have $\langle(\delta N)^2\rangle < \langle N\rangle$, which is called *sub-Poissonian* or *anti-bunched*. Thus, we get the important result that the noise is indicative of statistics. However, one should be careful to consider, when analyzing a system, all additional effects and correlations that can change the statistics of fluctuations. For example, in resonance fluorescence in optics it turns out that the photons are anti-bunched (the atom cannot emit a photon before absorbing another one, so there is a time lag that separates the photons); also blockade mechanisms can create bunched fermions.

IV. SCATTERING METHOD APPLIED TO NOISE

The scattering method is a powerful tool to noise calculations. I will present here a sketch of the main ideas, following [4]. The emphasis is mostly to understanding the final result and its applications. Additional details about the derivation can be found in the textbooks.

We will use the second-quantization (quantum) version of scattering theory. The current fluctuation operator is

$$\delta\hat{I}_\alpha(t) = \hat{I}_\alpha(t) - \langle\hat{I}_\alpha\rangle, \tag{37}$$

and the aim is to calculate

$$S_{\alpha\beta}(t'-t) = \langle\langle\delta\hat{I}_\alpha(t)\delta\hat{I}_\beta(t') + \delta\hat{I}_\beta(t')\delta\hat{I}_\alpha(t)\rangle, \tag{38}$$

and we get for the Fourier transform

$$S_{\alpha\beta}(\omega) = \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} S_{\alpha\beta}(\tau). \tag{39}$$

Note that in other places $S_{\alpha\beta}(t'-t)$ is defined with a factor of $1/2$ in front (to reflect the fact that we symmetrized the correlation). We now use the expression for the current in the scattering formalism, as derived in the lecture on scattering theory,

$$\hat{I}_\alpha = \frac{e}{h}\sum_{\beta\gamma}\sum_{m,n}\int dE\int dE' e^{i(E-E')t/\hbar}\hat{a}^\dagger_{\beta m}(E)A^{\beta\gamma}_{mn}(\alpha;E,E')\hat{a}_{\gamma n}(E'), \tag{40}$$

where we introduced the notation

$$A^{\beta\gamma}_{mn}(\alpha;E,E') = \delta_{mn}\delta_{\alpha\beta}\delta_{\alpha\gamma} - \sum_k (\mathbf{s}^{\alpha\beta}_{mk})^\dagger(E)\mathbf{s}^{\alpha\gamma}_{kn}(E'). \tag{41}$$

At this point we have not separated the spin index: it is easier to do this later, at the end of the calculation. We now employ Wick's theorem (written for fermions only - the bosonic case is similar):

$$\langle \hat{a}^\dagger_{\alpha k}(E_1)\hat{a}_{\beta l}(E_2)\hat{a}^\dagger_{\gamma m}(E_3)\hat{a}^\dagger_{\delta n}(E_4)\rangle - \langle \hat{a}^\dagger_{\alpha k}(E_1)\hat{a}_{\beta l}(E_2)\rangle\langle \hat{a}^\dagger_{\gamma m}(E_3)\hat{a}^\dagger_{\delta n}(E_4)\rangle \tag{42}$$

$$= \delta_{\alpha\delta}\delta_{\beta\gamma}\delta_{kn}\delta_{ml}\delta(E_1 - E_4)\delta(E_2 - E_3)f_\alpha(E_1)[1 - f_\beta(E_2)]. \tag{43}$$

Using this expression we get

$$S_{\alpha\beta}(\omega) = \frac{e^2}{h}\sum_{\gamma\delta}\sum_{mn}\int dE A^{\gamma\delta}_{mn}(\alpha; E, E+\hbar\omega)A^{\delta\gamma}_{nm}(\beta; E, E+\hbar\omega) \times \tag{44}$$

$$\times \left\{ f_\gamma(E)[1 - f_\delta(E+\hbar\omega)] + [1 - f_\gamma(E)]f_\delta(E+\hbar\omega) \right\}. \tag{45}$$

The positive- and negative- frequencies are related to each other by $S_{\alpha\beta}(\omega) = S_{\beta\alpha}(-\omega)$.

Next, we focus on the zero-frequency noise, $\omega = 0$,

$$S_{\alpha\beta}(0) = S_{\beta\alpha}(0) = \frac{e^2}{h}\sum_{\gamma\delta}\sum_{mn}\int dE A^{\gamma\delta}_{mn}(\alpha; E, E)A^{\delta\gamma}_{nm}(\beta; E, E) \times \tag{46}$$

$$\times \left\{ f_\gamma(E)[1 - f_\delta(E)] + [1 - f_\gamma(E)]f_\delta(E) \right\}. \tag{47}$$

We will now consider a two-terminal device, and apply the general result Eq. (47). In this case, as we discussed in the scattering theory lecture, we have the representation:

$$\begin{pmatrix} \hat{b}_{L1} \\ ... \\ \hat{b}_{LN_L} \\ \hat{b}_{R1} \\ ... \\ \hat{b}_{RN_R} \end{pmatrix} = \mathbf{s} \begin{pmatrix} \hat{a}_{L1} \\ ... \\ \hat{a}_{LN_L} \\ \hat{a}_{R1} \\ ... \\ \hat{a}_{RN_R} \end{pmatrix}. \tag{48}$$

A similar expression holds for $\hat{a}^\dagger$ and $\hat{b}^\dagger$ but with the matrix $\mathbf{s}^\dagger$. The matrix $\mathbf{s}$ has dimensions $(N_L + N_R) \times (N_L + N_R)$ and it has the representation

$$\mathbf{s} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix}. \tag{49}$$

The dimensions of the reflection matrix r is $(N_L \times N_L)$, that of r' is $(N_R \times N_R)$ of t is $(N_R \times N_L)$, and of t' is $(N_L \times N_R)$. We now replace the indices α, β with L and R to obtain

$S = S_{LL} = S_{RR} = -S_{LR} = -S_{RL}$ and

$$S = \frac{2e^2}{h} \int dE \left\{ Tr[A^{LL}(E)A^{LL}(E)](f_L(E)(1-f_L(E)) + \right. \tag{50}$$

$$+Tr[A^{RR}(E)A^{RR}(E)]f_R(E)(1-f_R(E)) + \tag{51}$$

$$\left. +Tr[A^{LR}(E)A^{RL}(E)][f_L(E)(1-f_R(E)) + f_R(E)(1-f_L(E))] \right\} \tag{52}$$

Next, we use the definition Eq. (41) in the expression above. Note also that $r^\dagger r = I - t^\dagger t$. The matrix $t^\dagger t$ is then diagonalized (the same procedure as in the lecture on scattering theory) and the transmission eigenvalues of $t^\dagger t$ are denoted, as in the scattering lecture, by T_n. We find

$$Tr[r^\dagger r t^\dagger t] = \sum_n T_n(1-T_n). \tag{53}$$

It is now also time to separate the spin from the summation, so from now on we will take the index n as not including the spin. Because we are left with a single summation, this means that we just have to add a factor of two in front of the expression of noise. With these, we can find a reasonably compact formula for the noise derived in the scattering approach for two terminals,

$$S = 2\frac{2e^2}{h} \sum_n \int dE \left\{ T_n(E)[f_L(E)(1-f_L(E)) + f_R(E)(1-f_R(E))] + \right. \tag{54}$$

$$\left. + T_n(E)[1-T_n(E)][f_L(E) - f_R(E)]^2 \right\}. \tag{55}$$

If we now assume that the transmission probabilities do not change much with energy around the Fermi level, that is $T_n(E) \approx T_n(E_F) = T_n$, we can integrate [6] over energies and get our final formula

$$S = 2\frac{2e^2}{h} \left[2k_{\rm B}T \sum_n T_n^2 + eV \coth\left(\frac{eV}{2k_{\rm B}T}\right) \sum_n T_n(1-T_n) \right], \tag{56}$$

where V is the voltage difference between the L and R leads. As an additional observation, note that perturbation theory applied to this problem would fail to account for the terms in T_n^2 present in the formula above.

You might wonder how to derive Eq. (56), which is a very compact and elegant result while the integrals over the Fermi function seem terribly complicated. Integrals of Fermi functions are called Fermi integrals and some appear quite often in solid-state problems. You can find a list in Appendix A7 of the textbook [1], and we have also have discussed some in the Appendix of Lecture 1.

Here these two integrals are useful:

$$\int_0^\infty dE f_R(1-f_L) = \frac{\mu_L - \mu_R}{e^{\frac{\mu_L-\mu_R}{k_B T}} - 1}, \tag{57}$$

$$\int_0^\infty dE (f_L - f_R) = \mu_L - \mu_R. \tag{58}$$

To evaluate the integral over $(f_L - f_R)^2$ we use the following trick: we write

$$(f_L - f_R)^2 = -f_L(1-f_L) - f_R(1-f_R) + f_L(1-f_R) + f_R(1-f_L), \tag{59}$$

and we use the integrals listed above to find

$$\int_0^\infty dE (f_L - f_R)^2 = (\mu_L - \mu_R) \coth \frac{\mu_L - \mu_R}{2k_{\rm B}T} - 2k_{\rm B}T. \tag{60}$$

You can now use these expressions to obtain indeed Eq. (56).

We can now analyze the two limits of this expression.

A. Thermal noise

The expression for thermal (Johnson-Nyquist) noise can be obtained from Eq. (56) in the limit $eV \ll k_{\rm B}T$; we find

$$S = 2\frac{2e^2}{h} 2k_{\rm B}T \sum_n T_n = 4K_{\rm B}TG, \tag{61}$$

where $G = (2e^2/h)\sum_n T_n$ is the Büttiker conductivity derived previously. Thus, thermal noise is related to conductance (a consequence, as mentioned above, of the fluctuation-dissipation theorem) and as a result we cannot find any new information from the noise (more than from just conductance measurements).

• To understand a bit better how this came about, we can look one step back in Eq. (55). If the system is in thermal equilibrium, then $f_R = f_L = f$ and only the first term in that equation survives. We can use the relation

$$f(1-f) = k_B T \left(-\frac{\partial f}{\partial E}\right). \tag{62}$$

Recall now that we proved the Landauer formula for the conductance in the form

$$G = 2\frac{e^2}{h} \sum_n \int dE T_n(E) \left(-\frac{\partial f(E-\mu)}{\partial E}\right). \tag{63}$$

Inserting these expressions in Eq. (55), we get

$$S = 4k_B T G, \tag{64}$$

which is the Nyquist-Johnson noise.

B. Shot noise

We now look at the zero-temperature case and a finite voltage bias V applied to the leads $\mu_L - \mu_R = eV$. From Eq. (56) we have

$$S = 2\frac{2e^3V}{h}\sum_n T_n(1-T_n), \tag{65}$$

which is a rather general formula for the shot noise.

• We can also look back in Eq. (55) to understand where this comes from. At $T = 0$ the product $f(1-f)$ vanishes and we are left with

$$S = 2\frac{e^2}{h}\sum_n \int_{\mu_L}^{\mu_R} dE T_n(E)[1-T_n(E)]. \tag{66}$$

If we now assume that the tunnel probabilities are constant and with $\mu_R - \mu_L = eV$ we get indeed

$$S = 2\frac{2e^3V}{h}\sum_n T_n(1-T_n), \tag{67}$$

Poissonian limit

In the limit $T_n \ll 1$ we can recover our previous result Eq. (70) for the Poissonian current fluctuations. Indeed, Eq. (65) in the limit $T_n \ll 1$ yields

$$S_P = 2\frac{2e^3V}{h}\sum_n T_n = 2eGV = 2e\langle I\rangle, \tag{68}$$

where we used the Landauer-Büttiker result $G = 2(e^2/h)\sum_n T_n$. which is the same as

$$\langle I\rangle = \frac{e}{\Delta t}\langle N\rangle = e\Gamma, \tag{69}$$

$$S_P = \frac{2e}{\Delta t}\langle(\delta N)^2\rangle = 2e^2\Gamma = 2e\langle I\rangle. \tag{70}$$

Fano factor

We have defined the Fano factor as

$$F = \frac{S}{2e\langle I\rangle}, \tag{71}$$

so we can immediately calculate it with the equations above.

Alternative forms of this formula can be obtained by recall again the Landauer conductance formula $G = 2(e^2/h)\sum_n T_n$ and $\langle I\rangle = GV$. This results in the following expression for the Fano factor, which is often encountered in the literature,

$$F = \frac{\sum_n T_n(1-T_n)}{\sum_n T_n}. \tag{72}$$

The factor $(1 - T_n)$, which appears in each channel, always reduces the overall noise. Thus $F \leq 1$ (sub-Poissonian noise), as expected for noninteracting electrons.

V. EXAMPLES

The results obtained above are general, valid for conductors and elastic scattering. Now for any system, once we know the transmission probabilities T_n, we can calculate the Fano factor.

A. Single tunnel junction

In the case of the tunnel junction, the transmission probability is small, $T_n \ll 1$. In this case we get directly from Eq. (56) that the noise is

$$S = 2\frac{2e^3V}{h} \coth\left(\frac{eV}{2k_BT}\right) \sum_n T_n = \coth\left(\frac{eV}{2k_BT}\right) S_P. \tag{73}$$

where for the last equality we used $G = 2e^2/h \sum_n T_n$ and $\langle I \rangle = GV$. This illustrates in a compact form the cross-over between thermal noise ($k_BT \gg e|V|$) and shot noise ($k_BT \ll e|V|$). This crossover has been demonstrated experimentally, for example using STMs [7], see Fig. (V A).

B. Quantum point contact

The quantum point contact is defined by a saddle constriction of the type

$$V(x, y) = V_0 - \frac{1}{2}m\omega_x^2 x^2 + \frac{1}{2}m\omega_y^2 y^2, \tag{74}$$

for which the transmission probability (Büttiker) can be obtained for which the transmission probability can be obtained

$$T_n(E) = \frac{1}{1 + e^{-2\pi(E-\epsilon_n)/\hbar\omega_x}}. \tag{75}$$

where

$$\epsilon_n = \left[\hbar\omega_y \left(n + \frac{1}{2}\right) + V_0\right]. \tag{76}$$

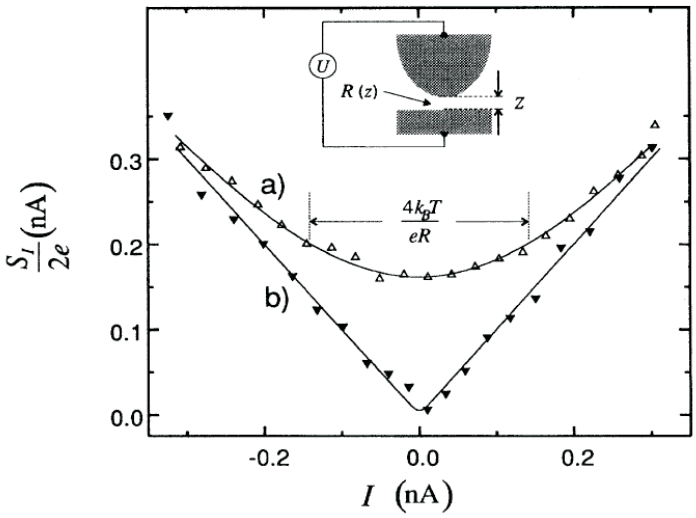

FIG. 1. Crossover between thermal and shot noise in an STM experiment. The solid lines are the prediction of Eq. (73). a) corresponds to T = 300 K and b) corresponds to T = 77 K. Figure from Ref. [7].

This expression for the transmission can be substituted into Eq. (66), and therefore for $E = E_{\rm F}$ we can calculate the noise as a function of the difference $E_{\rm F} - V_0$ (which is set experimentally by the gate voltage, which controls the number of conducting channels see Fig. V B). The result is that the shot noise has a strong peak at each conductance step. This has also been confirmed experimentally.

C. Diffusive wires

The result is $F = \frac{1}{3}$. This comes from the following considerations: for these wires the transmission distribution ρ_D (the number of channels that have a given transmission T) is known,

$$\rho_D = \frac{\langle G \rangle}{2G_Q} \frac{1}{T\sqrt{1-T}}, \tag{77}$$

where $G_Q = \frac{2e^2}{h}$ is the quanta of conductance. For example, the total number of channels is $\int_0^1 dT \rho_D$. To convince yourself that this distribution is consistent with the Landauer formula, calculate

$$\langle G \rangle = G_Q \int_0^1 dT \rho_D T. \tag{78}$$

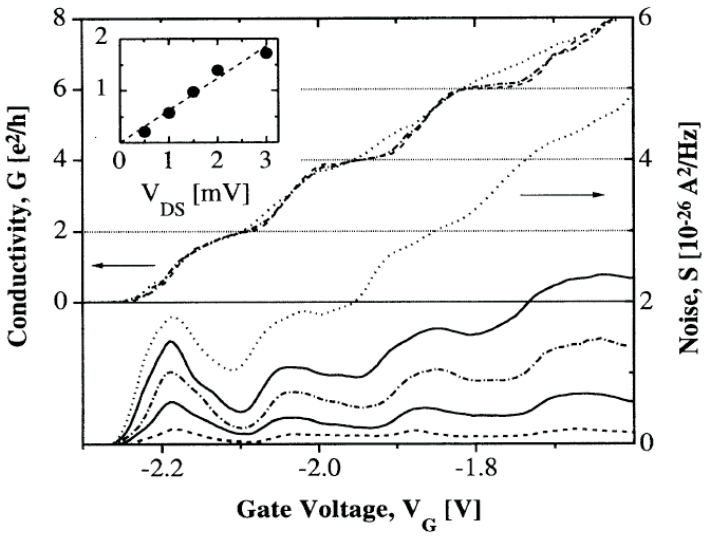

FIG. 2. Normalized conductivity and noise spectral density for a point contact versus the gate voltage $V_{\rm G}$. Figure from Ref. [8].

The Fano factor is obtained from the formula Eq. (72),

$$F = \frac{\int_0^1 dT \rho_D T(1-T)}{\int_0^1 dT \rho_D T} = \frac{1}{3}. \tag{79}$$

where the integrals can be calculated by a simple substitution $x = \sqrt{1-T}$.

D. Chaotic cavities

Chaotic cavities are ballistic systems with irregular shape and with scattering only at the surface. They are connected to the leads by small point contacts that result in a number N_L and N_R of open channels at the left and the right lead. The noise for chaotic cavities can be calculated and the Fano factor turns out to be

$$F = \frac{N_L N_R}{N_L + N_R}. \tag{80}$$

VI. HOW TO MEASURE NOISE

The simplest setup to measure would use a cold amplifier and a room-temperature amplifier; at the end of the measurement chain, the detector is a nonlinear element (to provide a reading of $(\delta I)^2$), which is recorded in a computer. The whole measurement chain needs

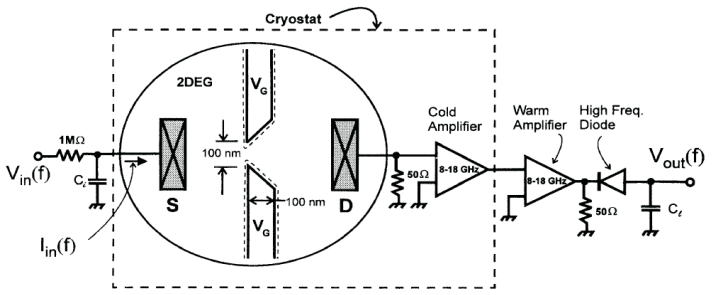

FIG. 3. In this setup, the current is modulated at a low frequency $f < 1kHz$ and the amplified excess noise, synchronous with f, is measured using a lock-in technique. The modulation and lock-in detection improve the signal-to-noise ratio. The current and its high-frequency fluctuations are amplified in the band $8 - 18$ GHz and detected by a high-frequency diode which provides an output $V_{\rm out}(f) \approx \langle (\delta I)^2 \rangle_{10\rm GHz}$. Figure from Ref. [8].

to be carefully calibrated with a known sample (*e.g.* a resistor). For example, in Fig. VI we present the measurement setup used for taking the data from Fig. V B.

Further readings: a number of excellent review are available in you want to learn more, [3–5].

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[1] Tero T. Heikkilä, The physics of nanoelectronics, Oxford University Press (2013), Chapter 2.

[2] Yuli. V. Nazarov and Yaroslav M. Blanter, Quantum Transport - Introduction to Nanoscience, Cambridge University Press, Cambridge (2009), Chapter 1.

[3] M. J. M. de Jong and C. W. J. Beenakker, Shot Noise in mesoscopic systems, preprint cond-mat/9611140.

[4] Ya. M. Blanter and M. Büttiker, Shot Noise in Mesoscopic Conductors, Phys. Rep. **336**, 1 (2000), arXiv:cond-mat/9910158.

[5] C. Beenakker and C. Schönenberger, Quantum Shot Noise, Physics Today, May 2003, 37, arXiv:cond-mat/0605025.

[6] M. Büttiker, Phys. Rev. B **46**, 12485 (1992); Th. Martin and R. Landauer, Phys. Rev. B **45**, 1742 (1992).

[7] Phys. Rev. Lett. **75**, 1610 (1995).

[8] M. Reznikov, M. Heiblum, H. Shtrikman, and D. Mahalu, Phys. Rev. Lett. **75**, 3340 (1995).

Elements of scattering theory

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Abstract

PHYS-E0551 Low Temperature Physics: Nanoelectronics

I. INTRODUCTION

This lecture introduces a number of essential concepts in quantum transport, related to the scattering formalism and the so-called Landauer-Büttiker approach. This is a very versatile approach with countless applications in transport phenomena in solids. It does not include inelastic effects, but it does include (unlike the Bolzmann approach) interference effects. The main assumption in the theory is that the system (a wire for example) is connected to large reservoirs. All the inelastic processes happen in the reservoir, while in the wire the electrons flow unimpeded (ballistically). In this way, the problem is reduced to a standard quantum-mechanical scattering problem.

To motivate the discussion and set the problem, let us look at how we describe in electronics the flow of a current through an ohmic conductor of resistance R when a voltage V is applied. We write for the current the Ohm's law $I = RV$, without worrying about the microscopic description of the electrons' flow in the conductor. We then calculate the resistance as $R = \rho L/S$, where ρ is the resistivity, L the length, and S the transversal area. If we now make $S \to 0$, we formally get $R \to \infty$: - this would imply that narrowing down the transversal area S of a conductor, the conductance goes smoothly to zero. In reality, this is not what is seen in experiments: the conductance decreases in steps, which are quantized in units of a quantum of conductance $G_Q = 2e^2/h$. The quantity $G_K = e^2/h = 3.8 \times 10^{-5}\Omega^{-1}$, which is half the quantum of conductance, and corresponds to a resistance $R_K = G_K^{-1} = 25.8$ kΩ is also important in the integer quantum Hall effect, where the transversal conductance of a Hall sample has plateaus at integer multiples of G_K. The subscript K comes from the name of Klaus von Klitzing.

The essential concepts to be introduced in this lecture are:

- Transmission probabilities, denoted by T. The reflection is $R = 1 - T$. These probabilities are quantum-mechanical, thus they originate from a transmission amplitude t, with $T = tt^* = |t|^2$, and a reflection amplitude r, with $R = rr^* = |r|^2$.
- Ballistic conductors and channels: the transport occurs with transmission probability close to 1 - there is no scattering.
- Transversal modes.
- Scattering matrices.

- The Landauer-Büttiker formulation of transport.

II. TRANSVERSE MODES

We will model the wire conductors as waveguides with a finite width and thickness (x and y-directions) and an infinite length in the z-direction. We write the time-independent Schrödinger equation for the electrons in the wire as

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + U(x,y,z)\right]\psi(x,y,z) = E\psi(x,y,z). \tag{1}$$

Let us try to simplify the problem: the simplest and most natural approximation is to take the potential $U(x,y,z)$ independent of the coordinate z (to avoid backscattering). This allows us to use the method of separation of variables to search for a solution in the form

$$\psi(x,y,z) = \chi(x,y)e^{ik_z z}, \tag{2}$$

which yields

$$\left[-\frac{\hbar^2}{2m}(\partial_x^2 + \partial_y^2) + U(x,y)\right]\chi(x,y) = \epsilon\chi_n(x,y). \tag{3}$$

Next, we should specify the lateral boundary conditions. Since there usually a work potential of a few eV is required to extract electrons out of the metal, we can use the rectangular box model potential - the electrons are confined laterally and their wavefunction vanishes at the edge,

$$\chi(0,y) = \chi(L_x,y) = \chi(x,0) = \chi(x,L_y) = 0, \tag{4}$$

with L_x and L_y the transversal dimensions of the wire. We then get for the eigenfunctions

$$\chi_n(x,y) = A_n \sin(k_{n_x}x)\sin(k_{n_y}y), \tag{5}$$

with $k_{n_x} = n_x\pi/L_x$, $k_y = n_y\pi/L_y$, and $n = (n_x, n_y)$ the mode index of the transversal wavefunction, corresponding to a transverse-mode eigenenergy

$$\epsilon_n = \frac{\hbar^2}{2m}(k_{n_x}^2 + k_{n_y}^2). \tag{6}$$

We can then write

$$E = \epsilon_n + \frac{\hbar^2 k_z^2}{2m}. \tag{7}$$

Conversely, suppose you are interested in what happens with particles with a given energy E. Then the corresponding wavenumbers will depend on which transversal mode the particles occupy,

$$k_z^{(n)} = \pm\sqrt{\frac{2m}{\hbar^2}(E-\epsilon_n)}. \tag{8}$$

The group velocity in the z-direction is by definition

$$v_z^{(n)} = \frac{1}{\hbar}\frac{dE}{dk_z^{(n)}} = \frac{\hbar k_z^{(n)}}{m}. \tag{9}$$

Note that only states with $E \geq \epsilon_n$ carry current, in other words $k_z^{(n)}$ must be real (evanescent waves with imaginary k_z do not carry current). For example, if we have a reservoir with a certain Fermi energy, only the transverse modes with transverse energy ϵ_n below the Fermi level can carry current. It is also convenient to define a function $M(E)$ which counts the number of modes with energy ϵ_n below E,

$$M(E) = \sum_n \theta(E-\epsilon_n), \tag{10}$$

where the function θ is the Heaviside step function (0 for negative values of the argument and 1 for positive values).

III. TRANSMISSION AND REFLECTION PROBABILITIES

To get an idea on how electrons scatter on potentials, let us calculate the probability of reflection and transmission for a standard rectangular potential as in Fig. (1)a,

$$U(z) = \begin{cases} U_0, & \text{if } 0 < z < d \\ 0, & \text{otherwise.} \end{cases} \tag{11}$$

For a given energy E we have waves propagating to the right or to the left, with $k_z^{(n)} = \pm\sqrt{\frac{2m}{\hbar^2}(E-\epsilon_n)}$. Therefore

$$\psi(x) = \begin{cases} e^{ik_z z} + r^{-ik_z z} & \text{if } z < 0, \\ be^{i\kappa z} + ce^{-i\kappa z} & \text{if } 0 < z < 0, \\ te^{ik_z z} & \text{if } d < z \end{cases} \tag{12}$$

where under the barrier the momentum vector is given by $\kappa = \sqrt{\frac{2m}{\hbar^2}(E-\epsilon_n-U_0)}$. Note that if $E < \epsilon_n + U_0$ then κ is imaginary (evanescent wavefunctions), and $T(E)$ can still be non-zero.

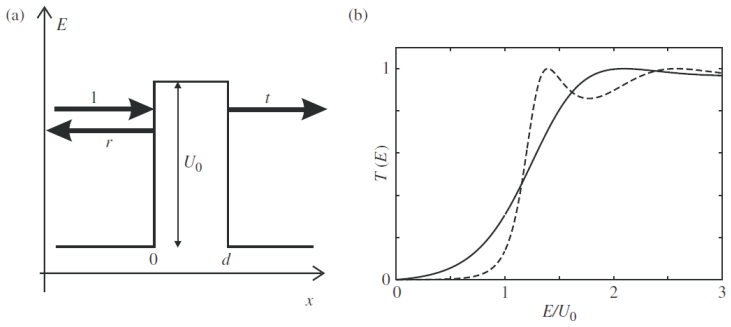

FIG. 1: a) Schematic of the barrier potential. b) $T(E)$ for $d\sqrt{2mU_0/\hbar^2}$ taking the value 3 (solid line) and 5 (dashed line). Figure from Ref. [2].

Transport happens in this situation by tunneling. From the continuity conditions (for the wavefunction and its first derivative) one can obtain, after some tedious but straightforward calculation,

$$T(E) = |t|^2 = \frac{4\kappa^2 k^2}{(k^2 - \kappa^2)\sin^2(\kappa d) + 4\kappa^2 k^2}, \tag{13}$$

and $R(E) = 1 - T(E)$. The transmission coefficient is plotted in Fig. (1)b.

Exercise: Show that if the energy E is well below the barrier, $T(E)$ becomes exponentially small in the width of the barrier. Discuss the connection with the WKB approximation.

IV. THE SCATTERING MATRIX

The scattering matrix offers a very compact form for calculating the transport properties, especially in the case of multiterminal devices. There are many reasons why this formalism is essential in nanoelectronics. The present nanotechnology techniques cannot produce perfectly identical structures; since these are nanoscale devices, changes and errors at the scale of a few atomic layers cannot be neglected as in the case of larger structures. Defects produce disorder and these are inevitably part of the device. Electrons scatter from these defects, and as a result the conductance depends on the exact distribution of disorder in the sample. It would be a tremendously difficult task to model all these effects.

However, if the scattering of electrons is lossless, it is possible to characterize the transport by a relatively small number of parameters. The idea is to identify several regions in the sample:

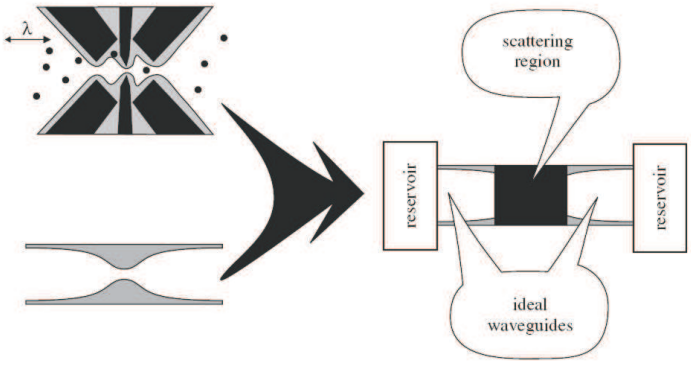

FIG. 2: Scattering approach to transport. A quantum point contact is modeled as a scattering region connected by waveguides to two reservoirs. Figure from Ref. [2].

(1) *The reservoirs* The reservoirs are assumed to be in thermal equilibrium and kept at a fixed voltage. We will call them "'left"(L) and "right" (R). The formalism can be easily generalized to several reservoirs.

(2) *The scattering region* This is the region where the "active" part of the nanostructure is placed.

(3) *The waveguides* These are the regions connecting the scattering region to the reservoirs.

In the waveguides, the wavefunction is a combination of plane waves, moving either in the positive-z direction or in the negative-z direction. We can write

$$\psi(x^L, y^L, z^L) = \sum_n \frac{1}{\sqrt{2\pi\hbar v_n}} \chi_n(x^L, y^L) \left[a_n^L e^{ik_z^{(n)} z^L} + b_n^L e^{-ik_z^{(n)} z^L} \right], \tag{14}$$

$$\psi(x^R, y^R, z^R) = \sum_m \frac{1}{\sqrt{2\pi\hbar v_m}} \chi_m(x^R, y^R) \left[a_m^R e^{-ik_z^{(m)} z^R} + b_m^R e^{ik_z^{(m)} z^R} \right]. \tag{15}$$

where n and m refers to the left- and respectively right- wavefunctions and

$$k_z^{(n)} = \pm\sqrt{\frac{2m}{\hbar^2}(E - \epsilon_n)}; \tag{16}$$

$$k_z^{(m)} = \pm\sqrt{\frac{2m}{\hbar^2}(E - \epsilon_m)}, \tag{17}$$

both real numbers (propagating not evanescent waves) corresponding to the same energy E. This condition limits the number of channels in the left- and right- waveguides to N_L and N_R (which are the maximum n and m such that $k_z^{(n)}$, $k_z^{(n)}$ are real).

Exercise: Note the normalization of these wavefunctions and calculate the corresponding particle current densities.

Clearly a_n^L, a_m^R are the amplitudes of the waves coming directly from the reservoirs and b_n^L, b_m^R are the amplitudes of the waves that interact with the scattering region. The scattering matrix connects these amplitudes,

$$b_l^\alpha = \sum_{\beta=L,R} \sum_p s_{lp}^{\alpha\beta} a_p^\beta, \quad \beta = L, R, \quad l = n, m, \tag{18}$$

or explicitly

$$b_l^\alpha = \sum_p s_{lp}^{\alpha L} a_p^L + \sum_p s_{lp}^{\alpha R} a_p^R, \quad l = n, m. \tag{19}$$

The scattering matrix $\hat{s}$ is simply a compact form for the coefficients $s_{lp}^{\alpha\beta}$,

$$\hat{s} = \begin{pmatrix} \hat{s}^{LL} & \hat{s}^{LR} \\ \hat{s}^{RL} & \hat{s}^{RR} \end{pmatrix} \sim \begin{pmatrix} \hat{r} & \hat{t}' \\ \hat{t} & \hat{r}' \end{pmatrix}. \tag{20}$$

The last equality defines four matrices. The $N_L \times N_L$ reflection matrix $\hat{r}$ describes the reflection of the waves from the left, while the $N_R \times N_R$ reflection matrix $\hat{r}'$ describes the reflection of the waves coming from the right. Similarly, the $N_R \times N_L$ matrix $\hat{t}$ and the $N_L \times N_R$ matrix $\hat{t}'$ describe the transmission through the structure.

Properties of the scattering matrix

a) Time-reversal symmetry. In the absence of a magnetic field we have time-reversal symmetry. This implies $\hat{s}^T = \hat{s}$ (T is transpose), and further $\hat{t}' = \hat{t}$ (or $t_{mn} = t'_{nm}$) as well as the symmetry of the reflection matrices, $r_{nn'} = r_{n'n}$ and $r'_{mm'} = r'_{m'm}$.

Exercise Write down the corresponding relations in the presence of a magnetic field B.

b) Unitarity. This is a consequence of conservation of the incoming and outgoing current.

We have $\hat{s}^\dagger \hat{s} = \hat{s}\hat{s}^\dagger = \hat{I}$. If we look at the diagonal elements,

$$(\hat{s}^\dagger \hat{s})_{nn} = \sum_{n'} |r_{nn'}|^2 + \sum_m |t_{mn}|^2 = 1. \tag{21}$$

Note now that

$$R_n = \sum_{n'} |r_{nn'}|^2 \tag{22}$$

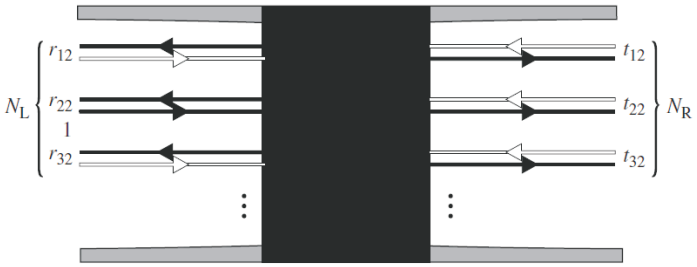

FIG. 3: The elements of the scattering matrix for $n' = 2$. Figure from Ref. [2].

is the probability for an electron in channel n to be reflected. The transmission probability is

$$T_n = \sum_m |t_{mn}|^2 = (\hat{t}^\dagger \hat{t})_{nn} = 1 - R_n. \tag{23}$$

Fig. (3) shows the matrix elements r_{n2} and t_{m2} for one left and one right lead.

V. THE LANDAUER-BÜTTIKER FORMALISM

A. Introduction

Let us now introduce the main idea by doing a very instructive calculation. The current that propagates in a wire of length L can be calculated by calculating the charge that passes through a surface in the $x - y$ plane per unit time, that is $2ev_z^{(n)}/L$, where n is the transversal mode. In other words, if we take into account only the states near the Fermi level (sometimes referred to as transport at the Fermi edge) the current can be calculated by taking two electrons (to include the spin degeneracy) per k_z-state and by summing over all modes near the Fermi level,

$$I^{(n)} = 2 \times \frac{e}{L} \sum_n v_z^{(n)} = 2 \times \frac{e}{L} \times \int \frac{dk_z}{2\pi/L} \frac{1}{\hbar} \frac{dE}{dk_z} = \frac{2e}{2\pi\hbar} \int_{E_F}^{E_F+eV} dE \frac{dE/dk_z}{dE/dk_z} = \frac{2e^2}{h} V, \tag{24}$$

where V is a bias voltage producing a displacement of the Fermi energy by eV. We used here the definition of $v_z^{(n)}$ from Eq. (9) and the relation $dk_z = (dk_z/dE)dE$.

This result is remarkably simple and beautiful. It shows that the conductance per longitudinal mode (channel) is simply

$$G_Q = \frac{2e^2}{h}. \tag{25}$$

If there are M channels open, the conductance will be $G = \frac{2e^2 M}{h}$. This is surprising: note that the result does not depend on the length of the wire, unlike what you would expect from the resistance formula $R = \rho L/S$.

We then move one step further to introduce the effect of the reservoirs and their filling factors. Consider now a cross-section though the left waveguide (see Fig. 2). The total current is a sum of three contributions: 1) electrons coming directly from the left reservoir ($k_z > 0$, filling factor f_L) moving to the right with speed v_z; 2) electrons that originate from the left reservoir and are reflected with probability $R_n(E) = \sum_{n'} |r_{n,n'}|^2$. These electrons carry a filling factor $f_L(E)$ and $k_z < 0$. 3) electrons coming from the right reservoir (filling factor $f_R(E)$ and $k_z < 0$) which are transmitted through the scattering region (probability $1 - R_n(E)$). So we just sum up these three contributions, again with a factor of 2 due to spin degeneracy,

$$I = 2\times e \sum_n \left\{ \int_0^\infty \frac{dk_z}{2\pi} v_z(k_z) f_L(E) + \int_{-\infty}^0 \frac{dk_z}{2\pi} v_z(k_z) R_n(E) f_L(E) + \int_{-\infty}^0 \frac{dk_z}{2\pi} v_z(k_z)(1 - R_n(E)) f_R(E) \right\} \tag{26}$$

Then, we change the variables $k_z \to -k_z$ (note that $v_z(-k_z) = -v_z(k_z)$) in order to get the same limits of the integral. Finally,

$$I = 2 \times e \sum_n \int_0^\infty \frac{dk_z}{2\pi} v_z(k_z) \left(1 - R_n(E)\right) \left[f_L(E) - f_R(E)\right]. \tag{27}$$

We now use the same trick as before: the magic of the density of states in 1-dimension which cancels up to a $\hbar$ the inverse of the velocity $v_z(k_z)$ works here as well,

$$I = 2 \times \frac{e}{h} \sum_n \int_0^\infty dE (1 - R_n(E)) \left[f_L(E) - f_R(E)\right]. \tag{28}$$

We then use the unitarity of the scattering matrix, which yields

$$1 - R_n = \sum_m |t_{mn}|^2 = (t^\dagger t)_{nn}, \tag{29}$$

therefore we can use the trace

$$\mathrm{Tr}\left[t^\dagger t\right] = \sum_n (t^\dagger t)_n, \tag{30}$$

to write

$$I = \frac{2e}{h} \int_0^\infty dE Tr\left[t^\dagger t\right] \left[f_L(E) - f_R(E)\right]. \tag{31}$$

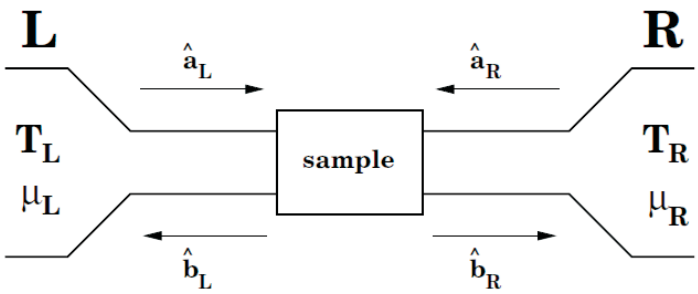

FIG. 4: Two-probe (two-terminal) scattering: the diagram shows the left and right reservoirs, the sample, and the left and right leads. Figure from Ref. [3].

This is our final result, called the Landauer formula. This formula allows us to calculate the conductance for many ballistic problems - from wires to graphene.

Exercise: Consider a zero-temperature Fermi distribution function for the two reservoirs, $f_L(E) = \theta(\mu_L - E)$ and $f_R(E) = \theta(\mu_R - E)$, where the difference in the chemical potentials is established by a bias voltage, $\mu_R - \mu_L = eV$. Calculate I using Eq. (31) and compare with the previous result Ref. (24).

B. Development of the formalism: second quantization

We now start to develop in a more rigurous way the Landauer-Büttiker formalism as a full quantum-mechanical theory of scattering. This can be done for an arbitrary number of leads, but most of the results presented here will aim at understanding the two-terminal problem (see Fig. V B). Generalizations to multiple terminals are relatively straightforward.

Wavefunctions in the scattering approach: momentum representation

The formalism starts with writing the wavefunction in the momentum representation, separating, as before, the incoming and outgoing components:

$$\Psi_\alpha(\vec{r},t) = \frac{1}{\sqrt{2\pi}} \sum_{n=1}^{N_{\alpha n}(E)} \int dk_{\alpha n} e^{-iE_{\alpha n}t/\hbar} \left[a_{\alpha n}(k_{\alpha n}) e^{ik_{\alpha n}z} + b_{\alpha n}(k_{\alpha n}) e^{-ik_{\alpha n}z} \right]. \qquad (32)$$

Second quantization

Next, we proceed to the second quantization picture in the standard way, by replacing the incoming and outgoing amplitudes with operators. These operators satisfy the usual

anticommutation relations. The same procedure will be used later in the course when we will discuss the quantization of transmission lines and scattering from cavities: in that case, the operators will be bosons and will satisfy (bosonic) commutation relations.

In momentum space, the canonical commutation relations are:

$$\left\{\hat{a}_{\alpha m}(k), \hat{a}^{\dagger}_{\beta n}(k')\right\} = \delta_{\alpha\beta}\delta_{nm}\delta_{k-k'}. \tag{33}$$

Note that because the indices must be equal, we don't have to write them each time for the vectors k, k'.

The introduction of second-quantized operators transforms Eq. (32) into a field operator,

$$\hat{\Psi}_{\alpha}(\vec{r}, t) = \frac{1}{\sqrt{2\pi}} \sum_{n=1}^{N_{\alpha n}(E)} \int dk_{\alpha n} e^{-iE_{\alpha n}t/\hbar} \left[\hat{a}_{\alpha n}(k_{\alpha n})e^{ik_{\alpha n}z} + \hat{b}_{\alpha n}(k_{\alpha n})e^{-ik_{\alpha n}z}\right]. \tag{34}$$

Energy representation

As usual in condensed matter physics, a more convenient representation is in terms of energy. To obtain this representation in the second quantization, we use the definitions of $k_{\alpha n}$ and $v_{\alpha n}$,

$$k_{\alpha n} = \frac{1}{\hbar}\sqrt{2m(E - E_{\alpha n})}, \tag{35}$$

and the velocity of the electrons in the n-th transverse channel is constructed from the momentum,

$$v_n(E) = \frac{\hbar k_{\alpha n}}{m}. \tag{36}$$

We thus have for example

$$dk_{\alpha n} = \frac{dE}{\hbar v_{\alpha n}}. \tag{37}$$

Now, we have to find the corresponding operators $\hat{a}_{\alpha n}(E)$ and $\hat{b}_{\alpha n}(E)$.

These operators have to satisfy

$$\{\hat{a}_{\alpha n}(E), \hat{a}^{\dagger}_{\beta m}(E')\} = \delta_{\alpha\beta}\delta_{mn}\delta(E - E'). \tag{38}$$

In order to find the relation between the momentum- and energy- representation operators, we use the delta-function relation

$$\delta(f(x)) = \sum_i \frac{1}{|\frac{df}{dx}(x_i)|}\delta(x - x_i), \tag{39}$$

where x_i are the roots of the equation $f(x) = 0$. So we then have

$$\delta(k-k') = \delta\left(\frac{\sqrt{2m}}{\hbar}\sqrt{E-E_{\alpha n}} - \frac{\sqrt{2m}}{\hbar}\sqrt{E'-E_{\alpha n}}\right) = \tag{40}$$

$$= \frac{1}{\hbar}\sqrt{\frac{m}{2(E-E_{\alpha n})}}\delta(E-E') = \tag{41}$$

$$= \frac{1}{\hbar v_{\alpha n}(E)}\delta(E-E'). \tag{42}$$

As a result, in order to have the proper commutation relations Eq. (38) we need to define the energy-representation creation and annihilation operators as

$$\hat{a}_{\alpha n}(E) = \frac{1}{\sqrt{\hbar v_{\alpha n}(k)}}\hat{a}_{\alpha n}(k). \tag{43}$$

$$\hat{a}^\dagger_{\alpha n}(E) = \frac{1}{\sqrt{\hbar v_{\alpha n}(k)}}\hat{a}^\dagger_{\alpha n}(k). \tag{44}$$

These results yield the following expression for the field operator in the energy representation

$$\hat{\Psi}_\alpha(\vec{r},t) = \int dE e^{-iEt/\hbar}\sum_{n=1}^{N_\alpha(E)}\frac{\chi_{\alpha n}(x,y)}{\sqrt{2\pi\hbar v_{\alpha n}(E)}}\left[\hat{a}_{\alpha n}(E)e^{ik_{\alpha n}(E)z} + \hat{b}_{\alpha n}(E)e^{-ik_{\alpha n}(E)z}\right], \tag{45}$$

therefore still composed of two waves (in-going and out-going) but with the operators depending on energy. Note that this is perfectly consistent with the expression of the wave function (in the first quantization) that we used before Eqs. (14,15).

Landauer current formula

With the field operator we can construct the current operator, using the standard quantum-mechanical definition,

$$\hat{I}_\alpha(z,t) = \frac{e\hbar}{2im}\int dxdy\left[\hat{\Psi}^\dagger_\alpha(\vec{r},t)\frac{\partial}{\partial z}\hat{\Psi}_\alpha(\vec{r},t) - \left(\frac{\partial}{\partial z}\hat{\Psi}^\dagger_\alpha(\vec{r},t)\right)\hat{\Psi}_\alpha(\vec{r},t)\right]. \tag{46}$$

We then insert the definition of the field operator Eq. (45) and using the orthogonality of the transverse wavefunctions $\chi_{\alpha n}$, that is

$$\int dxdy\chi^*_{\alpha n}(x,y)\chi_{\alpha m}(x,y) = \delta_{nm}, \tag{47}$$

and we obtain

$$\hat{I}_\alpha(z,t) = \int dEdE'\sum_n e^{i(E-E')t/\hbar}\frac{1}{2\pi\hbar\sqrt{v_{\alpha n}(E)v_{\alpha n}(E')}} \tag{48}$$

$$\Big\{(k_{\alpha n}(E)+k_{\alpha n}(E'))\left[\hat{a}^\dagger_{\alpha n}\hat{a}_{\alpha n}e^{i(k_{\alpha n}(E')-k_{\alpha n}(E))z} - \hat{b}^\dagger_{\alpha n}\hat{b}_{\alpha n}e^{i(k_{\alpha n}(E)-k_{\alpha n}(E'))z}\right] \tag{49}$$

$$+(k_{\alpha n}(E)-k_{\alpha n}(E'))\left[\hat{a}^\dagger_{\alpha n}\hat{b}_{\alpha n}e^{-i(k_{\alpha n}(E)+k_{\alpha n}(E'))z} - \hat{b}^\dagger_{\alpha n}\hat{a}_{\alpha n}e^{i(k_{\alpha n}(E)+k_{\alpha n}(E'))z}\right]\Big\} \tag{50}$$

We now assume that $k_{\alpha n}(E)$ and $v_{\alpha n}(E)$ are weakly dependent on energy, and we replace $v = \hbar k/m$ in the equation above. This results in a much simpler formula,

$$\hat{I}_\alpha(t) = \frac{e}{2\pi\hbar}\int dE dE' \sum_n e^{i(E-E')t/\hbar}\left[\hat{a}^\dagger_{\alpha n}(E)\hat{a}_{\alpha n}(E') - \hat{b}^\dagger_{\alpha n}(E)\hat{b}_{\alpha n}(E')\right]. \tag{51}$$

This equation has the following meaning: note $\hat{a}^\dagger_{\alpha n}(E)\hat{a}_{\alpha n}(E)$ is the particle number operator for incoming electrons and $\hat{b}^\dagger_{\alpha n}(E)\hat{b}_{\alpha n}(E)$ for the outcoming ones. Thus if we write $E' = E + \hbar\omega$ we see that the current is given by the difference between time-dependent occupation number operators of incoming and outgoing electrons. Note also that this quantity does not depend on z.

Scattering matrix for operators

In the same way as before, the idea is to describe the transport process entirely in terms of the scattering matrix s. This time however the amplitudes a and b will be promoted to quantum operators (second quantization). We then have for example in the case of two terminals

$$\hat{b} = S\hat{a}. \tag{52}$$

For the case of two terminals, with the leads L and R, we can write

$$\begin{pmatrix} \hat{b}_{L1} \\ ... \\ \hat{b}_{LN_L} \\ \hat{b}_{R1} \\ ... \\ \hat{b}_{RN_R} \end{pmatrix} = \mathbf{s} \begin{pmatrix} \hat{a}_{L1} \\ ... \\ \hat{a}_{LN_L} \\ \hat{a}_{R1} \\ ... \\ \hat{a}_{RN_R} \end{pmatrix}, \tag{53}$$

where the matrix s has dimension $(N_L + N_R) \times (N_L + N_R)$.

In general, with α and β labeling the reservoirs and with m a mode from reservoir β and n from reservoir α we have

$$\hat{b}_{\alpha n}(E) = \sum_{\beta,m} s^{\alpha\beta}_{nm}\hat{a}_{\beta m}, \tag{54}$$

$$\hat{b}^\dagger_{\alpha n}(E) = \sum_{\beta,m} \left(s^{\alpha\beta}_{nm}\right)^* \hat{a}^\dagger_{\beta m}. \tag{55}$$

If we insert these expressions in Eq. (51) we obtain

$$\hat{I}_\alpha(t) = \frac{e}{h}\int dEdE' \sum_j e^{i(E-E')t/\hbar}\left[\hat{a}^\dagger_{\alpha j}(E)\hat{a}_{\alpha j}(E') - \sum_{\beta\gamma}\sum_{mn}(s^{\alpha\beta}_{jm})^*(E)s^{\alpha\gamma}_{jn}(E')\hat{a}^\dagger_{\beta m}(E)\hat{a}_{\gamma n}(E')\right]. \tag{56}$$

This can be put in a more compact form

$$\hat{I}_\alpha(t) = 2\frac{e}{h}\sum_{\beta\gamma}\sum_{m,n}\int dE\int dE' e^{i(E-E')t/\hbar}\hat{a}^\dagger_{\beta m}(E)A^{\beta\gamma}_{mn}(\alpha;E,E')\hat{a}_{\gamma n}(E'), \tag{57}$$

where we added a factor of 2 for spin and we introduced the notation

$$A^{\beta\gamma}_{mn}(\alpha;E,E') = \delta_{mn}\delta_{\alpha\beta}\delta_{\alpha\gamma} - \sum_k(\mathbf{s}^{\alpha\beta}_{mk})^\dagger(E)\mathbf{s}^{\alpha\gamma}_{kn}(E'). \tag{58}$$

Finally, we can calculate the average current by using the Fermi distribution (we assume that the leads are in equilibrium), using the relation

$$\langle\hat{a}^\dagger_{\alpha m}(E)\hat{a}_{\beta n}(E')\rangle = \delta_{\alpha\beta}\delta_{mn}\delta(E-E')f_\alpha(E). \tag{59}$$

To simplify even more the result, we assume a two-terminal sample. In this case, the scattering matrix can be represented as

$$\mathbf{s} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix}. \tag{60}$$

The dimensions of the reflection matrix r is $(N_L \times N_L)$, that of r' is $(N_R \times N_R)$ of t is $(N_R \times N_L)$, and of t' is $(N_L \times N_R)$. The matrix $\mathbf{s}$ has dimensions $(N_L + N_R) \times (N_L + N_R)$. The matrix t is the off-diagonal block of the scattering matrix,

$$t_{mn} = \mathbf{s}^{RL}_{mn}. \tag{61}$$

As a result, we get

$$\langle I_L\rangle = 2\frac{e}{h}\int dETr[t^\dagger(E)t(E)][f_L(E) - f_R(E)]. \tag{62}$$

Another form of this expression is written by using the eigenvalues T_n of the matrix $t^\dagger t$, which are transmission probabilities. With these,

$$\langle I_L\rangle = 2\frac{e}{h}\int dE\sum_n T_n(E)[f_L(E) - f_R(E)]. \tag{63}$$

Linear response: Landauer conductance formula

Consider now the case when a small bias is applied to the device. We will get $\mu_L = \mu + eV/2$ and $\mu_R = \mu - eV/2$, where μ is the unbiased value. In the limit of small bias, with $f(E) = [1 + e^{E/k_BT}]^{-1}$ we get

$$f_L(E) - f_R(E) = f(E - \mu - eV/2) - f(E - \mu + eV/2) \approx eV \left(-\frac{\partial f(E-\mu)}{\partial E} \right). \quad (64)$$

Inserting in Eq. (63) we can readily find the conductance $\langle I_L \rangle = GV$,

$$G = 2\frac{e^2}{h} \sum_n \int dE T_n(E) \left(-\frac{\partial f(E-\mu)}{\partial E} \right). \quad (65)$$

For zero temperature, this becomes simply

$$G = 2\frac{e^2}{h} \sum_n T_n. \quad (66)$$

This formula is the Landauer conduction formula, now derived in the full quantum theory. The formula says that each quantum channel contributes with a unit of conductance $2e^2/h$ (again, 2 is the electron spin).

VI. EXAMPLE: THE QUANTUM POINT CONTACT

A quantum point contact (QPC) is narrow constriction (see Fig. VI)which allows the electrons to go through almost ballistically if the channel corresponds to a certain energy window. A good mathematical model (developed by Büttiker) is in terms of the potential

$$V(x, y) = V_0 - \frac{1}{2}m\omega_x^2 x^2 + \frac{1}{2}m\omega_y^2 y^2, \quad (67)$$

for which the transmission probability can be obtained

$$T_n(E) = \frac{1}{1 + e^{-2\pi(E-\epsilon_n)/\hbar\omega_x}}, \quad (68)$$

where

$$\epsilon_n = \left[\hbar\omega_y \left(n + \frac{1}{2} \right) + V_0 \right]. \quad (69)$$

Quiz: Note that the expression of $T_n(E)$ reminds of a step-like Fermi distribution function. What is the width of this step? What is the condition for the validity of $T_n(E) \approx \theta(E - \epsilon_n)$. A good approximation (see the quiz above) is

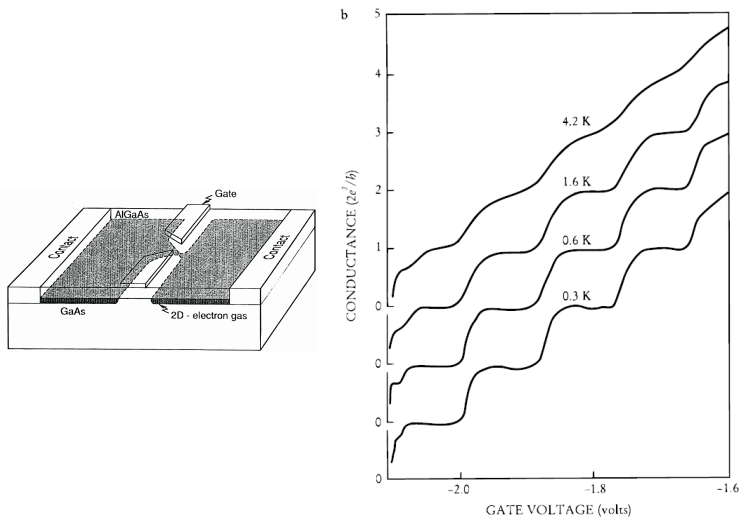

FIG. 5: Schematic of a quantum point contact formed when a negative voltage is applied to the gate electrodes on the top of the AlGaAs layer. This results in the creation of a potential of the type discussed above in the 2D electron gas of the interface of GaAs-AlGaAs junction. When the gate voltage made less negative, the number of propagating modes at the Fermi level increases stepwise. Figures from Ref. [4].

$$T_n(E) = \theta(E - \epsilon_n). \tag{70}$$

We now can calculate the conductivity using the formula Eq. (66),

$$G = 2\frac{e^2}{h}\sum_n \theta(E - \epsilon_n) = 2\frac{e^2}{h}N_L, \tag{71}$$

where N_L is the number of channels within the transport window.

This shows that the conductance is quantized in units of

$$\frac{2e^2}{h} = \frac{1}{12.5k\Omega} = 7.74 \times 10^{-5}\Omega^-1, \tag{72}$$

therefore each channel has a resistance of $12.5k\Omega$, a value which is easily measurable.

Indeed, what is seen in experiments is a sequence of conductance steps, as the gate voltage is increase and more and more modes are brought in the transport window.

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[1] Tero T. Heikkilä, The physics of nanoelectronics, Oxford University Press (2013), Chapter 3.

[2] Yuli. V. Nazarov and Yaroslav M. Blanter, Quantum Transport - Introduction to Nanoscience, Cambridge University Press, Cambridge (2009), Chapter 1.

[3] Ya. M. Blanter and M. Büttiker, Shot Noise in Mesoscopic Conductors, Phys. Rep. **336**, 1 (2000), arXiv:cond-mat/9910158.

[4] H. van Houten, and C.W.J. Beenakker, Physics Today, July 1996, page 22, cond-mat/0512609.