8.513 Lecture 3

Microscopic approach; Nonlocal transport; Voltage probes; Resonances

Derivation of Landauer formulas (multi-lead, multi-channel)

Second quantization summary

2.1.2 Second quantization

Fock space for fermions. Electrons are identical quantum-mechanical particles. To characterize a system of N (non-interacting) electrons, we have to consider Schrödinger equation for N particles. Assuming that the Hamiltonian is time independent, we look for the stationary solutions. They are products of the type

$$\psi(r_1 \dots r_N) = \psi_{i_1}(r_1)\dots\psi_{i_N}(r_N),$$

where i_k label all possible (single-particle) states of the Hamiltonian (the states with the different values of spin quantum number are counted as different, even though they are described with the same wave function in the absence of the magnetic field). Any linear combination of such products is also a solution.

The solutions are thus highly degenerate. This degeneracy is lifted if we take into account that electrons are fermions and obey the Pauli principle: In each quantum state i_k can be only one or zero electrons. Their wavefunction must be antisymmetric — it has to change sign every time we exchange two electrons.

To make it clear, let us consider an example of three free electrons. The (single-particle) quantum states are labeled by the wavevector $\boldsymbol{k}$ and the spin projection σ (which takes the values $\uparrow$ and $\downarrow$). We describe the many-particle state in which one electron is in the state $i_a = (\boldsymbol{k}\uparrow)$, one in the state $i_b = (\boldsymbol{k}\downarrow)$, and one in the state $i_c = (\boldsymbol{k}'\downarrow)$. The antisymmetric solution is

$$\psi(r_1, r_2, r_3) = \frac{1}{\sqrt{6}}\left[\psi_{i_a}(r_1)\psi_{i_b}(r_2)\psi_{i_c}(r_3) - \psi_{i_a}(r_1)\psi_{i_b}(r_3)\psi_{i_c}(r_2)\right.$$
$$+\psi_{i_a}(r_2)\psi_{i_b}(r_3)\psi_{i_c}(r_1) - \psi_{i_a}(r_2)\psi_{i_b}(r_1)\psi_{i_c}(r_3)$$
$$\left. + \psi_{i_a}(r_3)\psi_{i_b}(r_1)\psi_{i_c}(r_2) - \psi_{i_a}(r_3)\psi_{i_b}(r_2)\psi_{i_c}(r_1)\right],$$

with the corresponding energy $E = E_{i_a} + E_{i_b} + E_{i_c} = 2E_{i_a} + E_{i_c}$. Indeed, the permutation of two electrons, for instance, $r_1 \leftrightarrow r_2$, changes the sign of the wavefunction.

To implement systematically the Pauli principle, it is convenient to construct the *Fock space*. We begin with the space of all the solutions of the Schrödinger equation for N electrons, then combine all such spaces (including $N = 0$), and only keep the antisymmetric solutions (those compatible with the Pauli principle). An element of the Fock state $|n_1, n_2, \dots\rangle$ is labeled by the *occupation numbers* of the states 1, 2, … — zero if the state is empty and one if it is occupied. A special element

of the Fock state is vacuum — $|0, 0, \dots\rangle$ — when there are no particles in the system.

Creation and annihilation operators for fermions. The states of the Fock space can be obtained from the vacuum by application of a number of *creation operators*. The creation operator $\hat{a}_i^\dagger$ adds an electron into the state $|i\rangle$, described by the wavefunction $\psi_i(r)$.

$$\begin{aligned}\hat{a}_i^\dagger\,|n_1, \dots, n_{i-1}, 0, n_{i+1}, \dots\rangle &= \pm\,|n_1, \dots, n_{i-1}, 1, n_{i+1}, \dots\rangle,\\ \hat{a}_i^\dagger\,|n_1, \dots, n_{i-1}, 1, n_{i+1}, \dots\rangle &= 0,\end{aligned} \qquad (2.8)$$

where the sign depends on the sequence in which the states n_k were filled. The conjugated *annihilation operator* $\hat{a}_i$ takes an electron out of the same state,

$$\begin{aligned}\hat{a}_i\,|n_1, \dots, n_{i-1}, 1, n_{i+1}, \dots\rangle &= \pm\,|n_1, \dots, n_{i-1}, 0, n_{i+1}, \dots\rangle,\\ \hat{a}_i\,|n_1, \dots, n_{i-1}, 0, n_{i+1}, \dots\rangle &= 0.\end{aligned} \qquad (2.9)$$

These operators obey the anticommutation rules,

$$\begin{aligned}\left[\hat{a}_i^\dagger, \hat{a}_j\right]_+ &\equiv \hat{a}_i^\dagger\hat{a}_j + \hat{a}_j\hat{a}_i^\dagger = \delta_{ij}\ ;\\ \left[\hat{a}_i^\dagger, \hat{a}_j^\dagger\right]_+ &= [\hat{a}_i, \hat{a}_j]_+ = 0.\end{aligned} \qquad (2.10)$$

The operator $\hat{a}_i^\dagger\hat{a}_i$ describes the number of electrons in the state $|i\rangle$. Averaged over an arbitrary state A of the Fock space, it gives either one — if A contains a particle in $|i\rangle$ — or zero otherwise. In other words,

$$\langle\hat{a}_i^\dagger\hat{a}_i\rangle = n_i. \qquad (2.11)$$

The quantum-mechanical averages of all other products – $\langle\hat{a}_i^\dagger\hat{a}_j\rangle$ for $i \neq j$, $\hat{a}_i^\dagger\hat{a}_j^\dagger$, and $\hat{a}_i\hat{a}_j$ – equal zero.

Any operator can be expressed in terms of the creation and annihilation operators. For example, the Hamiltonian has the form,

$$\hat{H} = \sum_i E_i\hat{a}_i^\dagger\hat{a}_i, \qquad (2.12)$$

which just states that the total energy of the system is the sum of energies of all particles present in the system.

Field operators for fermions. Often rather than creation operators, which add a particle to a certain quantum state, it is convenient to use *field operators*, which create particles at a certain space point. The field operators are defined by

$$\hat{\psi}(r) = \sum_i \psi_i(r)\hat{a}_i; \quad \hat{\psi}^\dagger(r) = \sum_i \psi_i^*(r)\hat{a}_i^\dagger. \qquad (2.13)$$

from Nazarov & Blanter

Second quantization summary

The anticommutation rules for the creation and annihilation operators imply that the field operators obey the following relations,

$$\left[\hat{\psi}^\dagger(\boldsymbol{r}), \hat{\psi}(\boldsymbol{r}')\right]_+ = \delta(\boldsymbol{r}-\boldsymbol{r}'), \quad \left[\hat{\psi}^\dagger(\boldsymbol{r}), \hat{\psi}^\dagger(\boldsymbol{r}')\right]_+ = \left[\hat{\psi}(\boldsymbol{r}), \hat{\psi}(\boldsymbol{r}')\right]_+ = 0. \tag{2.14}$$

Again, all the operators can be expressed via the field operators. We give the expressions for the Hamiltonian,

$$\hat{H} = \int d\boldsymbol{r} \hat{\psi}^\dagger(\boldsymbol{r}) \left[-\frac{\hbar^2}{2m}\nabla^2 + U(\boldsymbol{r})\right] \hat{\psi}(\boldsymbol{r}), \tag{2.15}$$

charge density and current density operators,

$$\hat{\rho}(\boldsymbol{r}) = e\hat{\psi}(\boldsymbol{r})\hat{\psi}^\dagger(\boldsymbol{r}); \quad \hat{\boldsymbol{j}}(\boldsymbol{r}) = \frac{ie\hbar}{2m}\left[\hat{\psi}(\boldsymbol{r})\nabla\hat{\psi}^\dagger(\boldsymbol{r}) - (\nabla\hat{\psi}(\boldsymbol{r}))\hat{\psi}^\dagger(\boldsymbol{r})\right], \tag{2.16}$$

which look very similar to those derived in the usual Schrödinger equation description, but with the wave function replaced now by the field operator. This is why the description of quantum-mechanical particles with the wavefunction is referred to as the *first quantization*, and the description with the creation/annihilation or the field operators is called the *second quantization*.

An obvious advantage of the second quantization approach is that it authomatically takes into account statistical correlations betwen electrons due to the Pauli principle. Another advantage is that it easily incorporates *interactions* between electrons. Imagine that electrons interact via two-particle potential $V(\boldsymbol{r}-\boldsymbol{r}')$. This interaction term can be written as an operator,

$$\hat{V} = \frac{1}{2}\int d\boldsymbol{r}d\boldsymbol{r}' \hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}^\dagger(\boldsymbol{r}')V(\boldsymbol{r}-\boldsymbol{r}')\hat{\psi}(\boldsymbol{r}')\hat{\psi}(\boldsymbol{r}) \tag{2.17}$$

(the order of operators is important!!), which has to be added to the Hamiltonian of the non-interacting particles (2.15).

Bosons. Though the focus of this book is the transport of electrons, sometimes we deal with phonons and photons, which are bosons. We briefly therefore review the principles of second quantization for a system of bosons.

The many-body wavefunction of bosons is symmetric — it does not change when two electrons are exchanged. The Fock space is constructed in the same way as for fermions, but now the occupation numbers n_i in the state $|n_1, n_2, \ldots\rangle$ can assume all possible values $n_i = 0, 1 \ldots$.

The creation and annihilation operators for bosons, defined as

$$\begin{aligned} \hat{a}_i^\dagger |n_1, \ldots, n_i, \ldots\rangle &= \sqrt{n_i+1}\,|n_1, \ldots, n_i+1, \ldots\rangle, \\ \hat{a}_i |n_1, \ldots, n_i, \ldots\rangle &= \sqrt{n_i}\,|n_1, \ldots, n_i-1, \ldots\rangle, \end{aligned} \tag{2.18}$$

obey commutation, rather than anticommutation, rules,

$$\begin{aligned} \left[\hat{a}_i, \hat{a}_j^\dagger\right]_- &\equiv \hat{a}_i\hat{a}_j^\dagger - \hat{a}_j^\dagger\hat{a}_i = \delta_{ij}\ ; \\ \left[\hat{a}_i^\dagger, \hat{a}_j^\dagger\right]_- &= [\hat{a}_i, \hat{a}_j]_- = 0. \end{aligned} \tag{2.19}$$

The operator $\hat{a}_i^\dagger\hat{a}_i$ is the operator of the number of particles in the state i, and its quantum-mechanical average is the corresponding occupation number n_i.

The field operators are defined in the same way as for fermions, and obey the commutation relations,

$$\left[\hat{\psi}(\boldsymbol{r}), \hat{\psi}^\dagger(\boldsymbol{r}')\right]_- = \delta(\boldsymbol{r}-\boldsymbol{r}'), \quad \left[\hat{\psi}^\dagger(\boldsymbol{r}), \hat{\psi}^\dagger(\boldsymbol{r}')\right]_- = \left[\hat{\psi}(\boldsymbol{r}), \hat{\psi}(\boldsymbol{r}')\right]_- = 0. \tag{2.20}$$

All the operators are expressed via the field operators in the same way (2.15), (2.17) as for the case of fermions.

Heisenberg representation. So far, we have developed the second quantization approach in the *Schrödinger representation* — the wave function depends on time, and the operators are time independent. This is convenient as far as we are dealing with non-interacting particles in stationary potentials. If we have interaction between the particles or time-dependent fields, it is advantageous to shift the time dependence from the wave function to the operators. In this new *Heisenberg representation* the operators $\hat{A}_H$ are obtained from the corresponding operators in the Scrödinger representation, $\hat{A}_S$, by the following transformation,

$$\hat{A}_H(t) = e^{i\hat{H}t/\hbar}\hat{A}_S e^{-i\hat{H}t/\hbar}.$$

Differentiating this relation, we obtain the equations of motion for the operator $\hat{A}_H$,

$$i\hbar\frac{\partial \hat{A}_H}{\partial t} = \left[\hat{A}_H, \hat{H}\right]_-.$$

In particular, we write down the equations of motion for the field operators $\hat{\psi}^\dagger(\boldsymbol{r}, t)$, $\hat{\psi}(\boldsymbol{r}, t)$ in the Heisenberg representation. This is easy to do for non-interacting electrons,

$$i\hbar\frac{\partial\hat{\psi}^\dagger(\boldsymbol{r}, t)}{\partial t} = -\left(-\frac{\hbar^2}{2m}\nabla^2 + U(\boldsymbol{r})\right)\hat{\psi}^\dagger(\boldsymbol{r}, t);$$

from Nazarov & Blanter

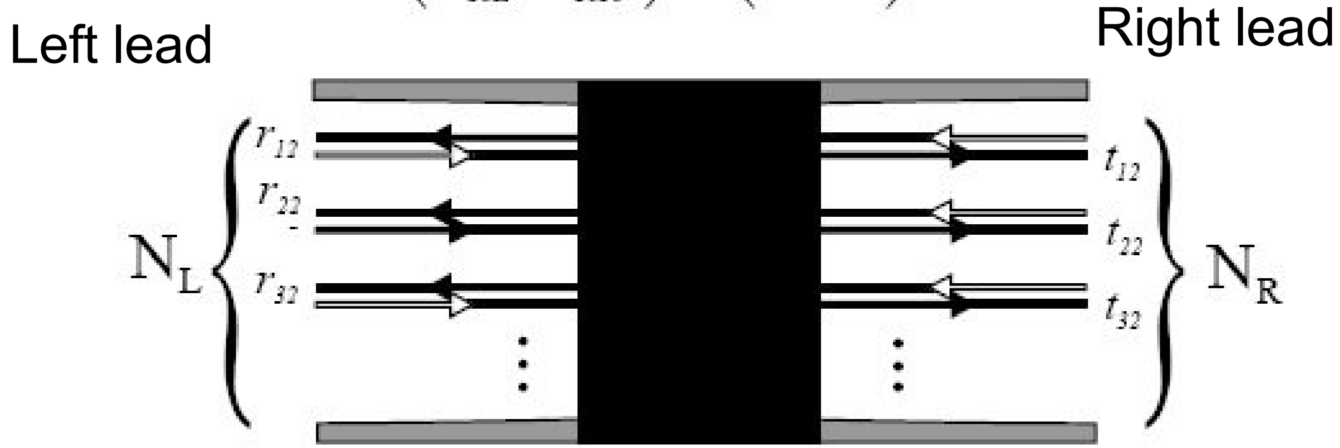
Second-quantized scattering states

$$\psi_{Ln}(x_L, y_L, z_L) = \frac{1}{\sqrt{2\pi\hbar v_n(E)}}\Phi_n(y_L, z_L)e^{ik_x^{(n)}x_L} + \sum_{n'} \frac{1}{\sqrt{2\pi\hbar v_{n'}(E)}} r_{n'n}(E)\Phi_{n'}(y_L, z_L)e^{-ik_x^{(n')}x_L},$$

$$\psi_{Ln}(x_R, y_R, z_R) = \sum_m \frac{1}{\sqrt{2\pi\hbar v_m(E)}} t_{mn}(E)\Phi_m(y_R, z_R)e^{-ik_x^{(m)}x_R}$$

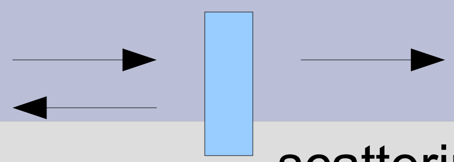
The proportionality coefficients are combined into a $(N_L + N_R) \times (N_L + N_R)$ *scattering matrix* $\hat{s}$. It has the following block structure,

$$\hat{s} = \begin{pmatrix} \hat{s}_{LL} & \hat{s}_{LR} \\ \hat{s}_{RL} & \hat{s}_{RR} \end{pmatrix} \equiv \begin{pmatrix} \hat{r} & \hat{t}' \\ \hat{t} & \hat{r}' \end{pmatrix}.$$

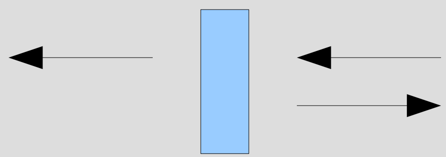


Operators for scattering states

A complete set:



scattering states

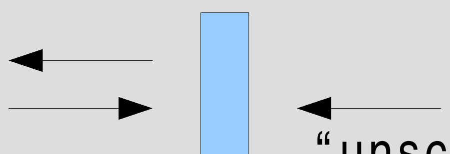


$$\psi_{Ln}(x_L, y_L, z_L) = \frac{1}{\sqrt{2\pi\hbar v_n(E)}}\Phi_n(y_L, z_L)e^{ik_x^{(n)}x_L} + \sum_{n'} \frac{1}{\sqrt{2\pi\hbar v_{n'}(E)}} r_{n'n}(E)\Phi_{n'}(y_L, z_L)e^{-ik_x^{(n')}x_L},$$

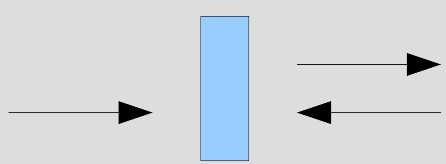
$$\psi_{Ln}(x_R, y_R, z_R) = \sum_m \frac{1}{\sqrt{2\pi\hbar v_m(E)}} t_{mn}(E)\Phi_m(y_R, z_R)e^{-ik_x^{(m)}x_R}$$

For each of these states, we can introduce creation and annihilation operators. Let us introduce the creation operators $\hat{a}^\dagger_{Ln}(E)$ and $\hat{a}^\dagger_{Rm}$ which create electrons in the scattering states with the energy E, originating from the left reservoir in the transport channel n, and from the right reservoir in the transport channel m, respectively. The conjugated operators $\hat{a}_{Ln}(E)$ and $\hat{a}_{Rm}$ annihilate particles in the same states. The operators $\hat{a}^\dagger$, $\hat{a}$ refer to a basis and therefore are sufficient for the quantum-mechanical description of the system.

An alternative complete set:



“unscattering” states



$$b_{\alpha l} = \sum_{\beta=L,R}\sum_{l'} s_{\alpha l,\beta l'} a_{\beta l'}, \quad \beta = L, R, \quad l = n, m.$$

However, for convenience we introduce another set of operators. The operator $\hat{b}^\dagger_{Ln}(E)$ creates an electron with the energy E in the transport channel n in the left waveguide moving to the left. A similar creation operator for right-movers in the right waveguide is $\hat{b}^\dagger_{Rm}(E)$, and the annihilation operators are $\hat{b}_{Ln}(E)$ and $\hat{b}_{Rm}(E)$. These operators are linarly related to the set $\hat{a}$ via the scattering matrix,

$$\hat{b}_{\alpha l}(E) = \sum_{\beta=L,R}\sum_{l'} s_{\alpha l,\beta l'}(E)\hat{a}_{\beta l'}(E);$$

$$\hat{b}^\dagger_{\alpha l}(E) = \sum_{\beta=L,R}\sum_{l'} s_{\beta l',\alpha l}(E)\hat{a}^\dagger_{\beta l'}(E), \quad \alpha = L, R, \quad l = n, m.$$

from Nazarov&Blanter

General properties

Anticommutation relations

$$\hat{a}^{\dagger}_{\alpha l}(E)\hat{a}_{\beta l'}(E') + \hat{a}_{\beta l'}(E')\hat{a}^{\dagger}_{\alpha l}(E) = \delta_{\alpha\beta}\delta_{ll'}\delta(E-E');$$
$$\hat{a}_{\alpha l}(E)\hat{a}_{\beta l'}(E') + \hat{a}_{\beta l'}(E')\hat{a}_{\alpha l}(E) = 0;$$
$$\hat{a}^{\dagger}_{\alpha l}(E)\hat{a}^{\dagger}_{\beta l'}(E') + \hat{a}^{\dagger}_{\beta l'}(E')\hat{a}^{\dagger}_{\alpha l}(E) = 0.$$

NB: operators *a* and *b* do not obey such relations!

Occupation numbers in reservoirs:

$$\left\langle \hat{a}^{\dagger}_{\alpha l}(E)\hat{a}_{\beta l'}(E') \right\rangle = \delta_{\alpha\beta}\delta_{ll'}\delta(E-E')f_{\alpha}(E), \quad \alpha = L, R.$$

Field operators that annihilate or create particle in the left lead

$$\hat{\Psi}(r,t) = \int dE e^{-iEt\hbar} \sum_n \frac{\Phi_n(y_L, z_L)}{\sqrt{2\pi\hbar v_n(E)}} \left[\hat{a}_{Ln} e^{ik_x^{(n)}x_L} + \hat{b}_{Ln} e^{-ik_x^{(n)}x_L}\right];$$
$$\hat{\Psi}^{\dagger}(r,t) = \int dE e^{iEt\hbar} \sum_n \frac{\Phi^*_n(y_L, z_L)}{\sqrt{2\pi\hbar v_n(E)}} \left[\hat{a}^{\dagger}_{Ln} e^{-ik_x^{(n)}x_L} + \hat{b}^{\dagger}_{Ln} e^{ik_x^{(n)}x_L}\right].$$

(similar for the right lead)

Current in the left lead

$$\hat{I}(x_L,t) = \frac{\hbar e}{2im} \int dy_L dz_L \left[\hat{\Psi}^{\dagger} \frac{\partial}{\partial x_L}\hat{\Psi} - \left(\frac{\partial}{\partial x_L}\hat{\Psi}^{\dagger}\right)\hat{\Psi}\right].$$

Electric current in the left lead

Sum over microscopic states in the leads

$$\hat{I}(x_L,t) = \frac{\hbar e}{2im}\int dy_L dz_L \left[\hat{\Psi}^\dagger \frac{\partial}{\partial x_L}\hat{\Psi} - \left(\frac{\partial}{\partial x_L}\hat{\Psi}^\dagger\right)\hat{\Psi}\right].$$

Imagine that all the quantities are periodic in time with the period $\mathcal{T} \to \infty$. from the condition that the exponents $\exp(iEt)$ periodic, $E = 2\pi q\hbar/\mathcal{T}$ with an integer q. Consequently, replace $\int dE$ by $2\pi\hbar/\mathcal{T}\sum_n$.

$$\left\langle e^{i(E-E')t}\right\rangle_t = \delta_{qq'} \text{ (time-average) and } \delta(E-E') \to \frac{\mathcal{T}}{2\pi\hbar}\delta_{qq'}.$$

Handle the continuum of states

$$\left\langle \hat{I}\right\rangle_t = \frac{G_Q}{e}\left(\frac{2\pi\hbar}{\mathcal{T}}\right)^2 \sum_n \sum_E \left[\hat{a}^\dagger_{Ln}(E)\hat{a}_{Ln}(E) - \hat{b}^\dagger_{Ln}(E)\hat{b}_{Ln}(E)\right].$$

Interpretation: current = # right-moving particles - # left-moving particles

$$\left\langle \hat{I}\right\rangle_t = \frac{G_Q}{e}\left(\frac{2\pi\hbar}{\mathcal{T}}\right)^2 \sum_n \sum_{\alpha\beta,ll'} \sum_E \hat{a}^\dagger_{\alpha l}(E)\hat{a}_{\beta l'}(E) \times \left[\delta_{\alpha L}\delta_{\beta L}\delta_{nl}\delta_{nl'} - s^*_{\alpha l,Ln}(E)s_{Ln,\beta l'}(E)\right].$$

(express *b*'s through *a*'s)

NB: this expression is still true for an arbitrary number of leads

Averaging over states in reservoirs

For two leads, using unitarity t^+t+r^+r=1, find

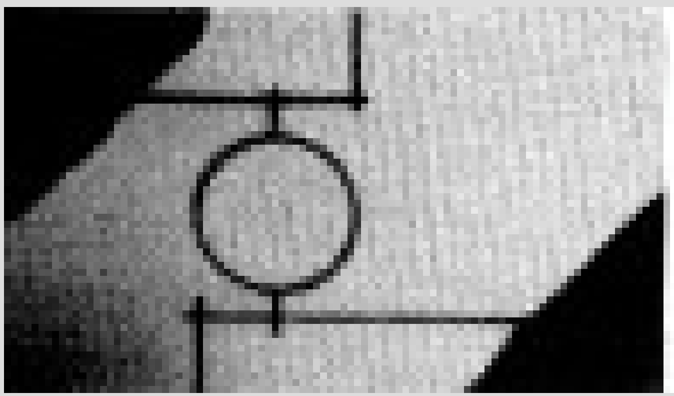
$$I = \frac{2_s e}{2\pi} \int_0^\infty dE \ \mathrm{Tr}\left[\hat{t}^\dagger \hat{t}\right] \left[f_L(E) - f_R(E)\right],$$

True for arbitrary energy distribution is reservoirs (T>0 etc), and for energy-dependent transmission T(ε)

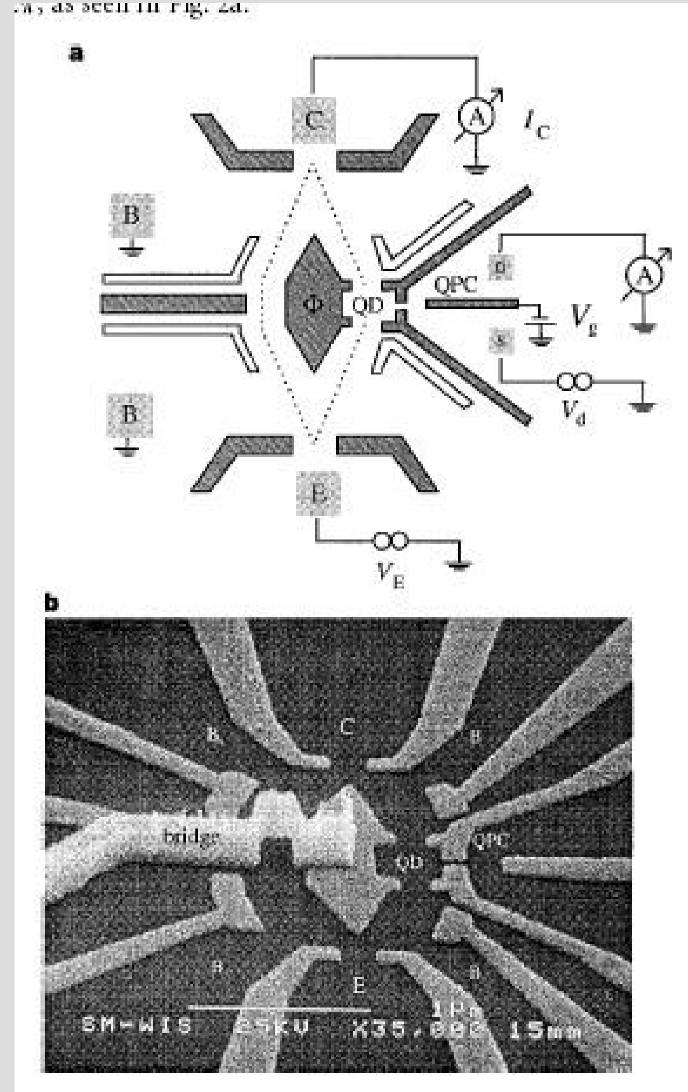
Taking V to zero get the Landauer formula

$$\mathrm{Tr}\left[\hat{t}^\dagger \hat{t}\right] = \sum_n \left(\hat{t}^\dagger \hat{t}\right)_{nn} . \qquad G = G_Q \sum_p T_p(E_F).$$

Multiterminal devices: rings, interferometers, etc



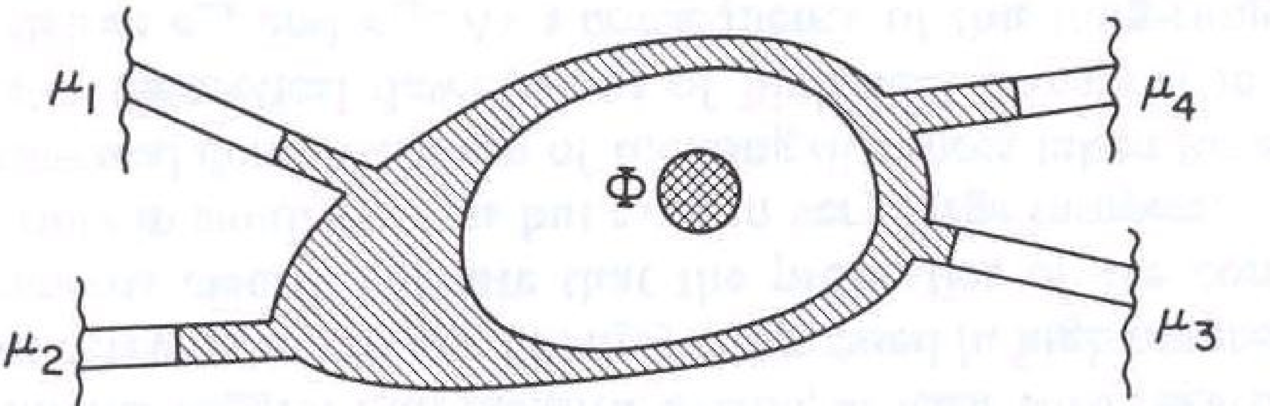
Webb et al. 1985



Heiblum et al. 1996

Multi-probe conductors

Buttiker, PRL 57, 1761 (1986); IBM J. Res. Developm. 32, 317 (1988)



$$\mu_\alpha = \mu_0 + eV_\alpha$$

$$I_\alpha = \frac{e}{h}\left[(N_\alpha - R_{\alpha\alpha})\,\mu_\alpha - \sum_{\beta\neq\alpha} T_{\alpha\beta}\,\mu_\beta\right]$$

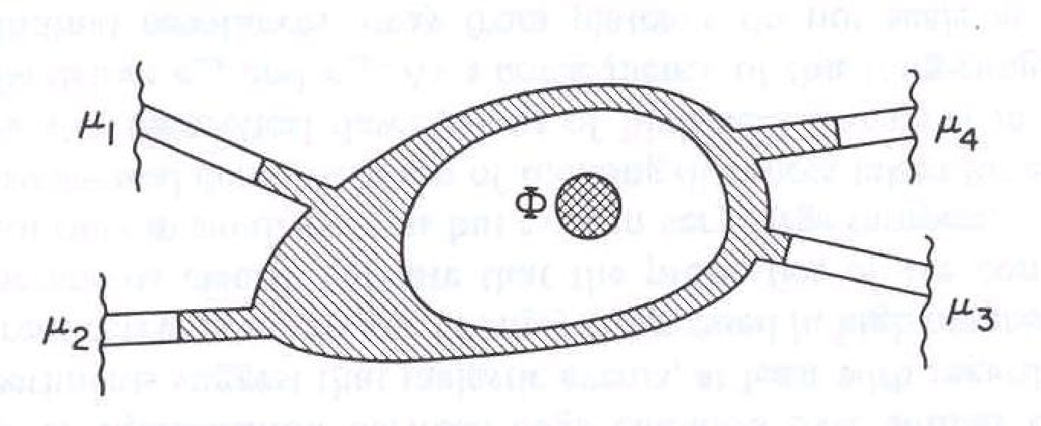
$$G_{\alpha\alpha} = dI_\alpha/dV_\alpha = \frac{e^2}{h}(N_\alpha - R_{\alpha\alpha}) = \frac{e^2}{h}\sum_{\beta\neq\alpha} T_{\alpha\beta}$$

$$G_{\alpha\beta} = dI_\alpha/dV_\beta = -\frac{e^2}{h} T_{\alpha\beta}$$

Quantum Kirchhoff law; current conservation; gauge invariance

$$I_\alpha = \sum_\beta G_{\alpha\beta} V_\beta \;; \quad \sum_\alpha G_{\alpha\beta} = 0 \;; \quad \sum_\beta G_{\beta\alpha} = 0$$

Multi-probe conductors: scattering matrix



$$s = \begin{pmatrix} s_{11} & s_{12} & s_{13} & s_{14} \\ s_{21} & s_{22} & s_{23} & s_{24} \\ s_{31} & s_{32} & s_{33} & s_{34} \\ s_{41} & s_{42} & s_{43} & s_{44} \end{pmatrix}$$

$$T_{\beta\alpha} = \sum_{mn} T_{\beta\alpha,mn} = \sum_{mn} |s_{\beta\alpha,mn}|^2 = Tr[s^\dagger_{\beta\alpha} s_{\beta\alpha}]$$

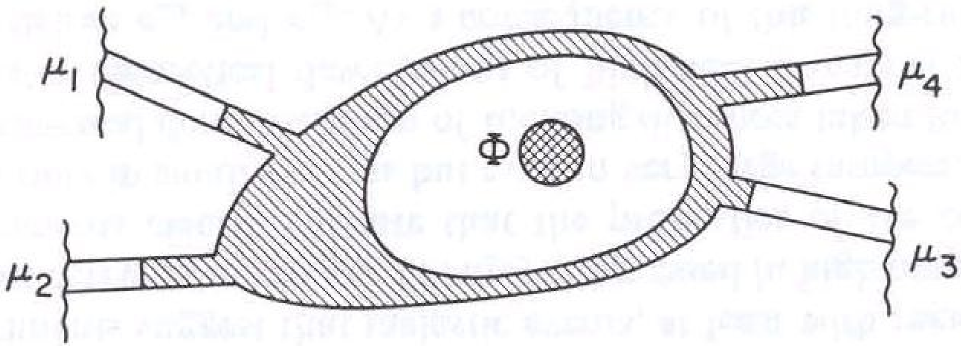
$$R_{\alpha\alpha} = \sum_{mn} R_{\alpha\alpha,mn} = \sum_{mn} |s_{\alpha\alpha,mn}|^2 = Tr[s^\dagger_{\alpha\alpha} s_{\alpha\alpha}]$$

magnetic field symmetry $s_{\beta\alpha,mn}(B) = s_{\alpha\beta,nm}(-B)$ $=$

$$T_{\alpha\beta}(B) = T_{\beta\alpha}(-B)\,;\;\; R_{\alpha\alpha}(B) = R_{\alpha\alpha}(-B)$$

$$G_{\alpha\beta}(B) = G_{\beta\alpha}(-B)\,;\;\; G_{\alpha\alpha}(B) = G_{\alpha\alpha}(-B)$$

Four-probe resistances



G has eigenvalue zero!

$$I_\alpha = \sum_\beta G_{\alpha\beta} V_\beta \; ; \quad \sum_\alpha G_{\alpha\beta} = 0 \; ; \quad \sum_\beta G_{\beta\alpha} = 0$$

$$I_\alpha = \frac{e}{h} \left[(N_\alpha - R_{\alpha\alpha})\, \mu_\alpha - \sum_{\beta \neq \alpha} T_{\alpha\beta}\, \mu_\beta \right]$$

Current contacts $I_\alpha = I \, , \; I_\beta = -I$

Voltage probes $I_\gamma = 0 \, , \rightarrow \; V_\gamma \, , \; I_\delta = 0 \, , \rightarrow \; V_\delta$

$$\mathcal{R}_{\alpha\beta,\gamma\delta} = \frac{V_\gamma - V_\delta}{I} = \frac{G_{\gamma\alpha} G_{\delta\beta} - G_{\gamma\beta} G_{\delta\alpha}}{\mathcal{D}}$$

$$\mathcal{R}_{\alpha\beta,\gamma\delta} = \frac{V_\gamma - V_\delta}{I} = \frac{h}{e^2} \frac{T_{\gamma\alpha} T_{\delta\beta} - T_{\gamma\beta} T_{\delta\alpha}}{D}$$

Voltage probes

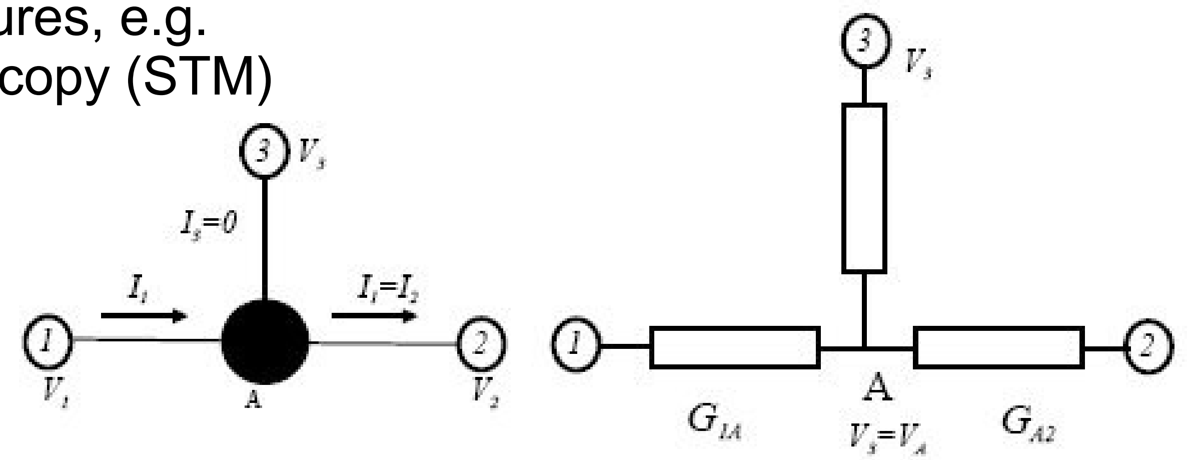
Voltage probes essential for electric circuits. What about quantum circuits?

An ideal probe: infinite resistance, thus non-invasive, does not perturb the distribution of currents in the tested circuit

Possible for nanostructructures, e.g. Scanning Tunneling Microscopy (STM)

However, interpreting results my be tricky b/c the laws of classical circuitry fail

Landauer-Buttiker three-terminal description of a voltage probe:



Three-terminal circuit with terminal 3 as a voltage probe. Right: A classical circuit could be presented in this way and conductances of the elements G_{1A}, G_{A2} can be determined from the voltage V_3 measured.

$$I_3 = G_{31}(V_1 - V_3) + G_{32}(V_2 - V_3), \qquad G_{33} = -G_{31} - G_{32}$$

this current has to be zero.

$$V_3 = \frac{G_{31}V_1 + G_{32}V_2}{G_{31} + G_{32}} = \frac{V_1 \mathrm{Tr}\ \hat{s}_{31}^{\dagger}\hat{s}_{31} + V_2 \mathrm{Tr}\ \hat{s}_{32}^{\dagger}\hat{s}_{32}}{\mathrm{Tr}\ \hat{s}_{31}^{\dagger}\hat{s}_{31} + \mathrm{Tr}\ \hat{s}_{32}^{\dagger}\hat{s}_{32}}$$

the voltage read by the voltmeter

In a classical circuit:

$$G_{1A} = G_{12}\frac{V_1 - V_2}{V_1 - V_3}; \quad G_{A2} = G_{12}\frac{V_2 - V_1}{V_2 - V_3}$$

Measurement is noninvasive if $G_{32}, G_{31} \ll G_{12}$

Scatterer with voltage probes

Apply to a single-lead scatterer (1D conductor)

Probe A, left lead:

the probability of tunneling into the voltage probe $w \ll 1$.

Contribution of reflected current:

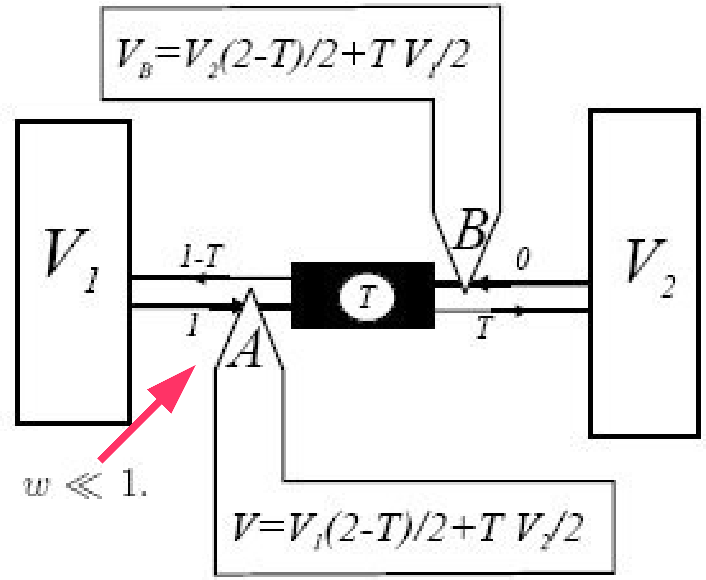
$$(1-w)(1-T)w \approx (1-T)w)$$

Voltage on Probe A:

$$V_A = V_1(1-T/2) + V_2 T/2.$$

Compare to classical relation

$$G_{1A} = G_{12}\frac{V_1 - V_2}{V_1 - V_3}; \quad G_{A2} = G_{12}\frac{V_2 - V_1}{V_2 - V_3}$$



$$G = G_Q T/(1-T) \ ?!$$

"Wrong" Landauer formula illustrates the non-local nature of conductance in nanostructures.

$$G_{1A} = G_{12}\frac{V_1 - V_2}{V_1 - V_A} = 2G_Q;$$

$$G_{AB} = G_{12}\frac{V_1 - V_2}{V_A - V_B} = G_Q\frac{T}{1-T};$$

$$G_{B2} = G_{12}\frac{V_1 - V_2}{V_B - V_2} = 2G_Q.$$

Series resistor representation

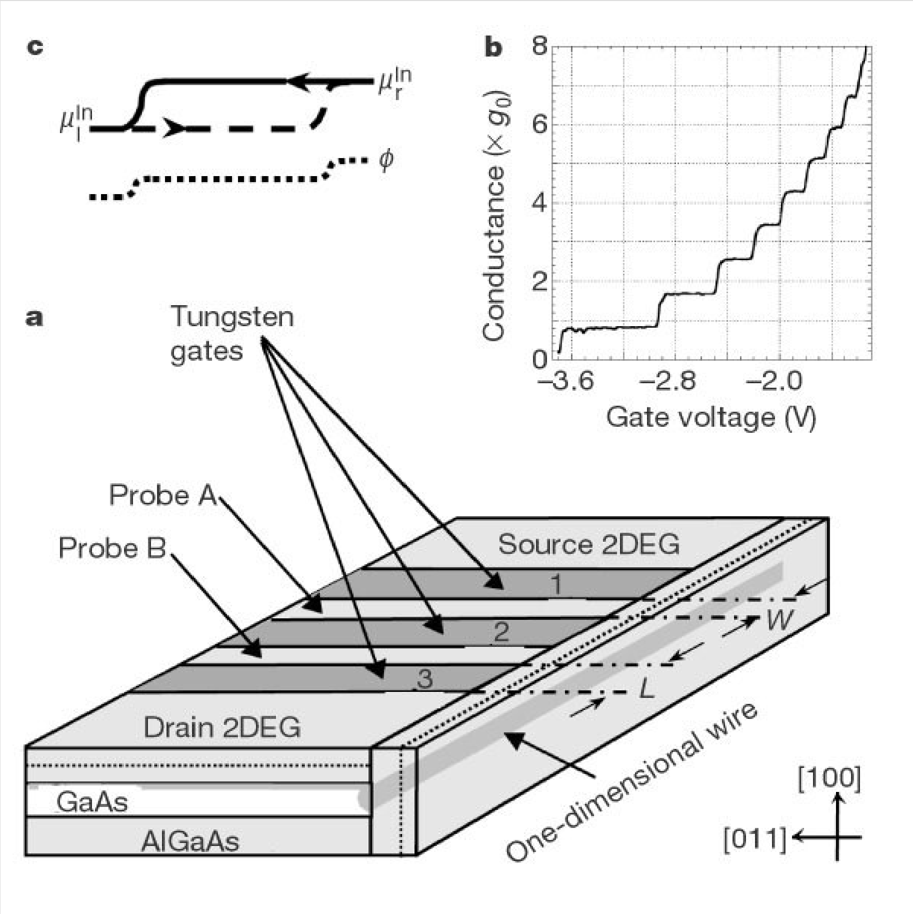
The "elements" with conductances $G_{1A} = G_{B2} = G_Q/2$ called contact resistance

T or T/(1-T)?

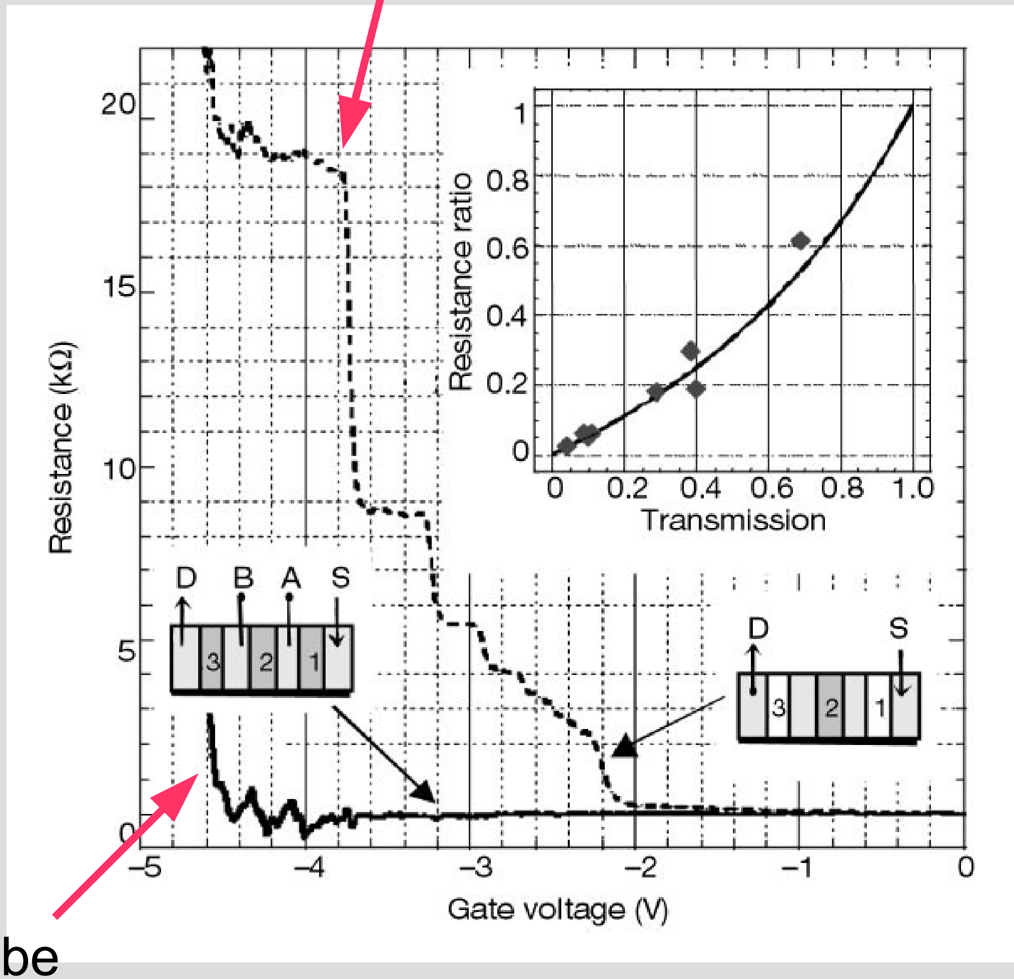
- Unexpected but no paradox, both formulas describe realistic but different situations
- Two-probe conductance T vs. four-probe conductance T/(1-T)
- Cannot **apply** voltage to a scatterer so that G=T/(1-T) b/c voltage in a quantum scatterer is applied to reservoirs, BUT can measure using voltage probes;
- Illustrates nonlocality of quantum transport

Experiment

Four-terminal resistance of a ballistic quantum wire,
de Picciotto et al. Nature 411, 51 (2001)

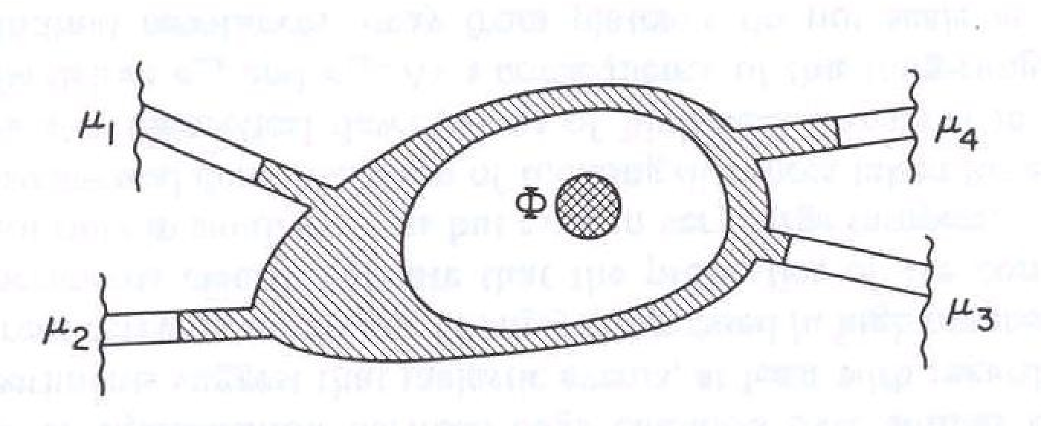


two-probe



four-probe

Multi-probe conductors: scattering matrix



$$s = \begin{pmatrix} s_{11} & s_{12} & s_{13} & s_{14} \\ s_{21} & s_{22} & s_{23} & s_{24} \\ s_{31} & s_{32} & s_{33} & s_{34} \\ s_{41} & s_{42} & s_{43} & s_{44} \end{pmatrix}$$

$$T_{\beta\alpha} = \sum_{mn} T_{\beta\alpha,mn} = \sum_{mn} |s_{\beta\alpha,mn}|^2 = Tr[s^\dagger_{\beta\alpha} s_{\beta\alpha}]$$

$$R_{\alpha\alpha} = \sum_{mn} R_{\alpha\alpha,mn} = \sum_{mn} |s_{\alpha\alpha,mn}|^2 = Tr[s^\dagger_{\alpha\alpha} s_{\alpha\alpha}]$$

magnetic field symmetry $s_{\beta\alpha,mn}(B) = s_{\alpha\beta,nm}(-B)$ $\Longrightarrow$

$$T_{\alpha\beta}(B) = T_{\beta\alpha}(-B)\,; \; R_{\alpha\alpha}(B) = R_{\alpha\alpha}(-B)$$

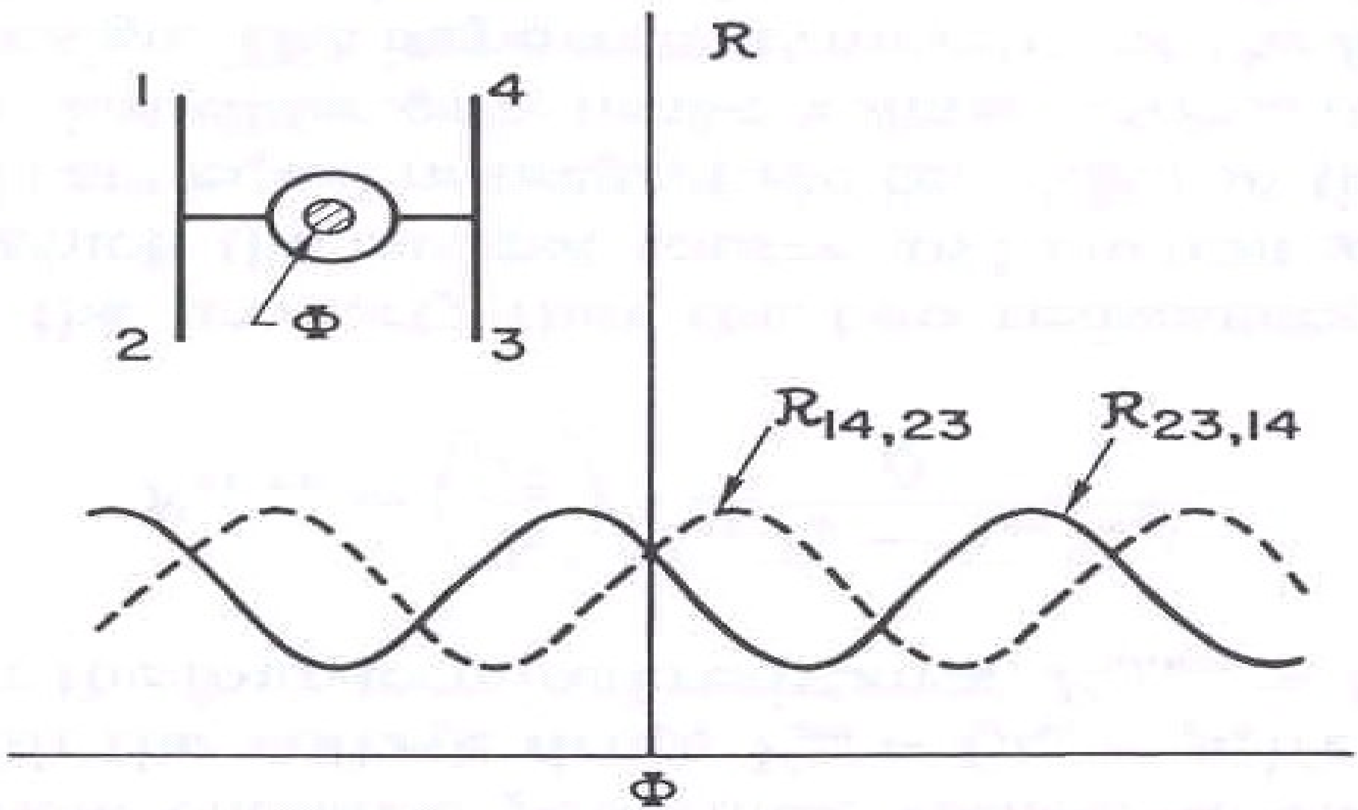
$$G_{\alpha\beta}(B) = G_{\beta\alpha}(-B)\,; \; G_{\alpha\alpha}(B) = G_{\alpha\alpha}(-B)$$

Reciprocity

$$\mathcal{R}_{\alpha\beta,\gamma\delta} = \frac{V_\gamma - V_\delta}{I} = \frac{h}{e^2}\frac{T_{\gamma\alpha}T_{\delta\beta} - T_{\gamma\beta}T_{\delta\alpha}}{D}$$

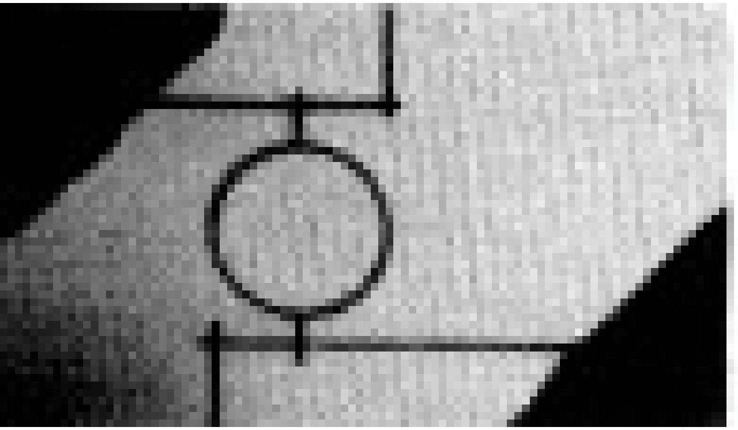
From $T_{\alpha\beta}(B) = T_{\beta\alpha}(-B)$ and $D(B) = D(-B)$

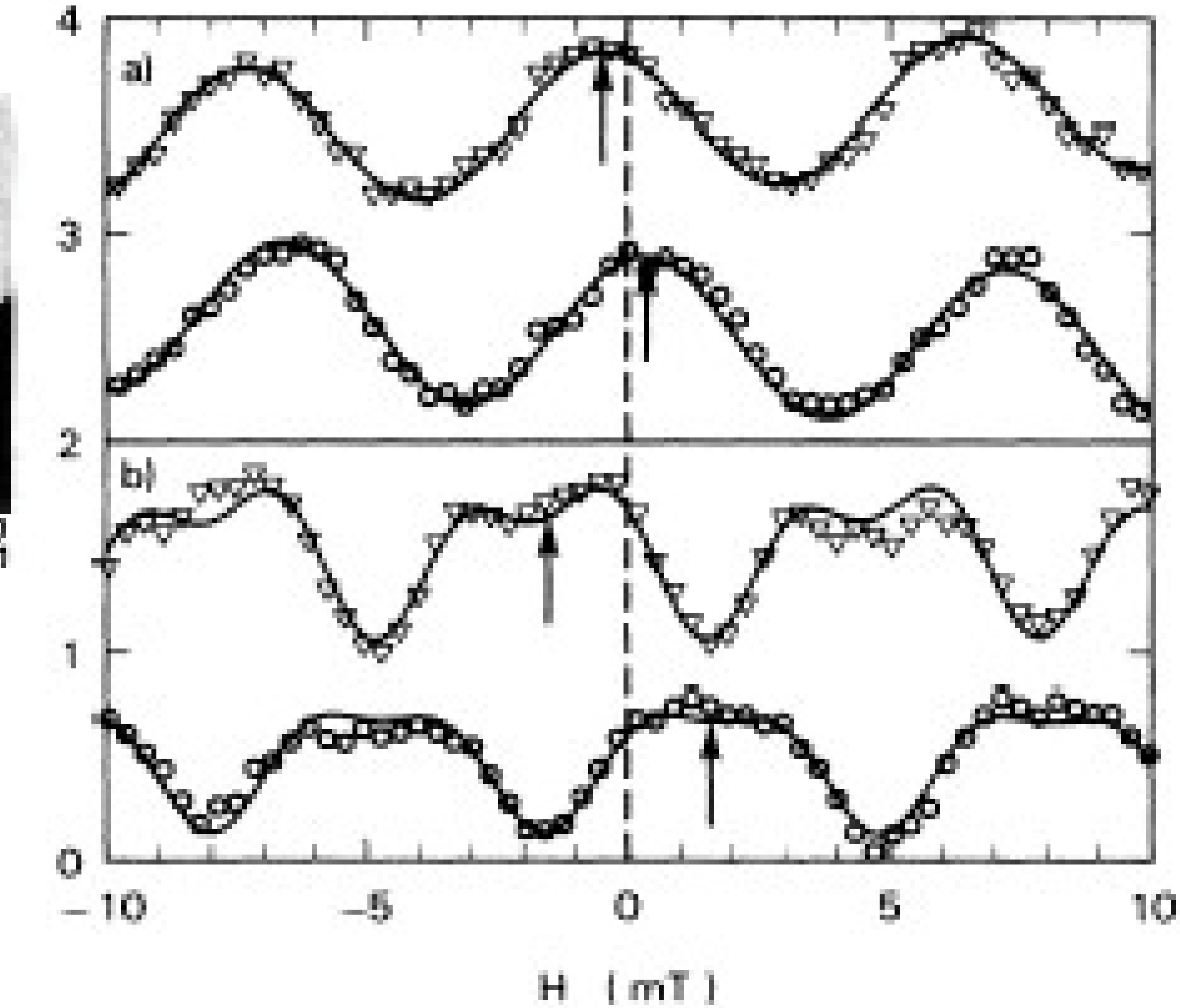
$$\mathcal{R}_{\alpha\beta,\gamma\delta}(\mathcal{B}) = \mathcal{R}_{\gamma\delta,\alpha\beta}(-\mathcal{B})$$



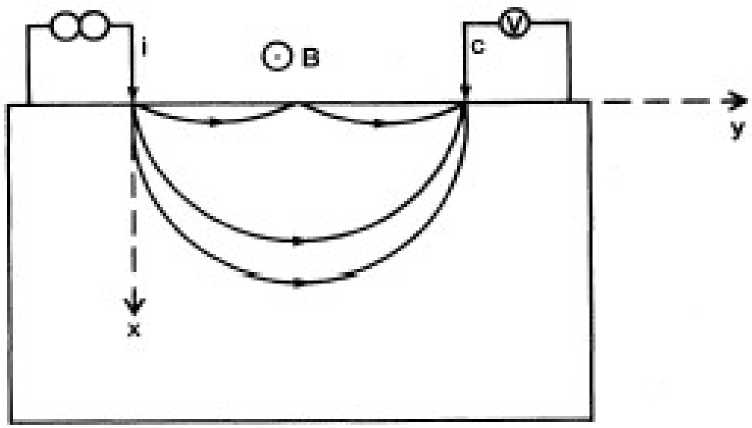
Reciprocity: Benoit et al.

Benoit, Washburn, Umbach, Laibowitz, Webb, PRL 57, 1765 (1986)





Reciprocity: van Houten et al.



$$\omega_c = |eB/mc|$$

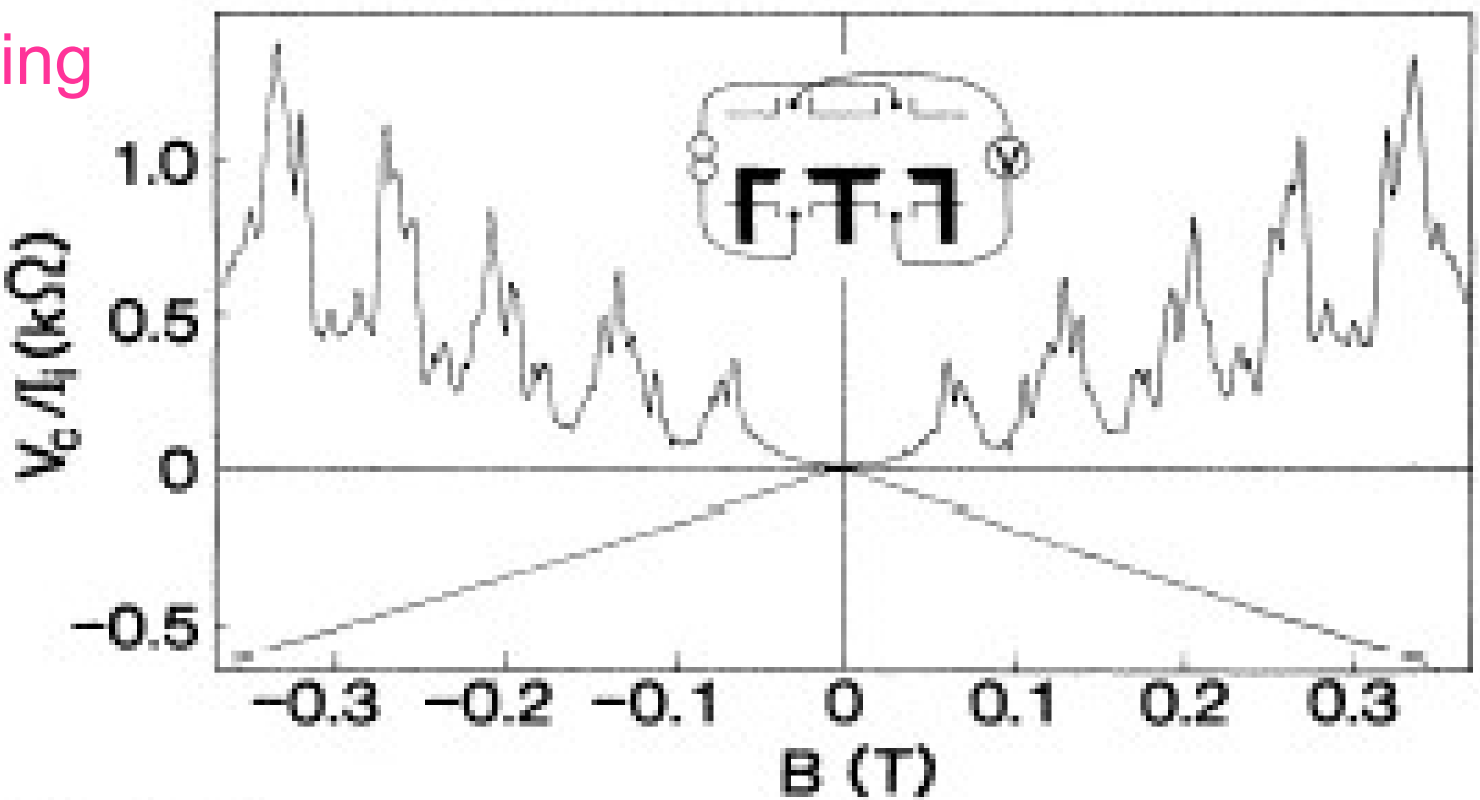
$$r_c \omega_c = v_F$$

$$r_c = c\, m\, v_F/|eB|$$

skipping orbit

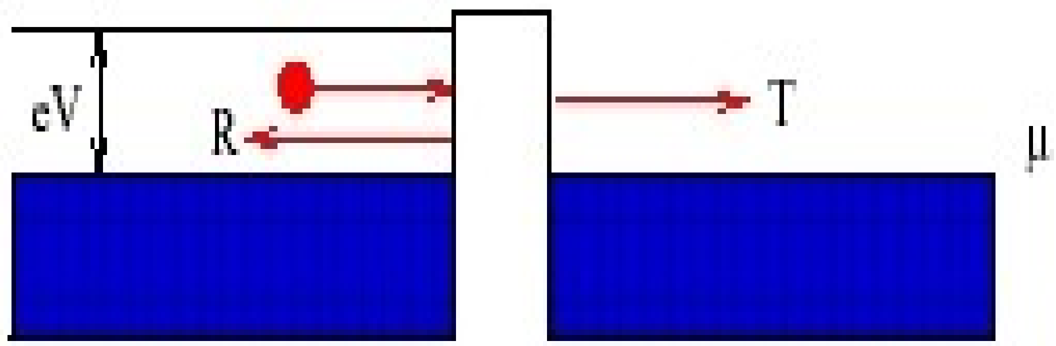
van Houten et al. , Phys. Rev. B39, 8556 (1989)

electron focusing



Microscopic derivation

Conductance from transmission



$$G = dI/dV = \frac{e^2}{h} T$$

conductance quantum $\frac{e^2}{h}$

$$\mathcal{R} = dV/dI = \frac{h}{e^2} \frac{1}{T}$$

resistance quantum

$$\frac{h}{e^2} \approx 24\, kOhm$$

dissipation and irreversibility

$$W = I\,V = G\,V^2$$

boundary conditions

Conductance: finite temperature

$$dI_{inc,L} = \frac{e}{h} dE\, f_L(E) \quad \Longrightarrow$$

current of left movers

$$I_L = \frac{e}{h} \int dE\, T(E)\, f_L(E)$$

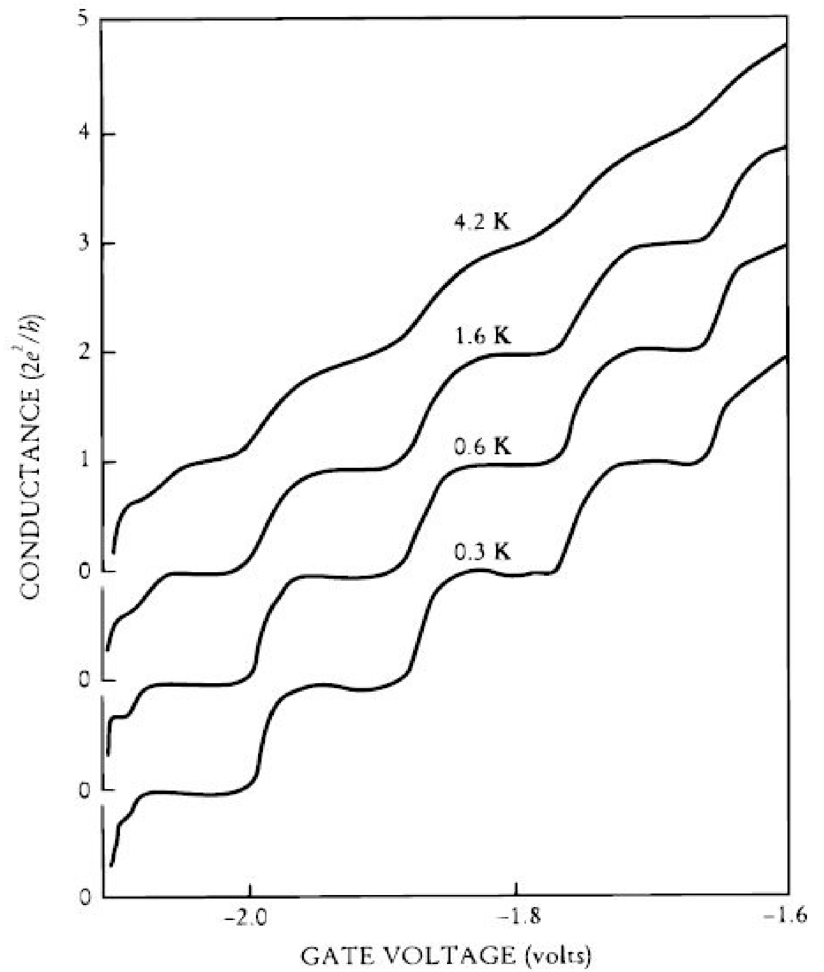
current of right movers

$$I_R = -\frac{e}{h} \int dE\, T(E)\, f_R(E)$$

net current

$$I = \frac{e}{h} \int dE\, T(E)\, (f_L(E) - f_R(E))$$

linear response



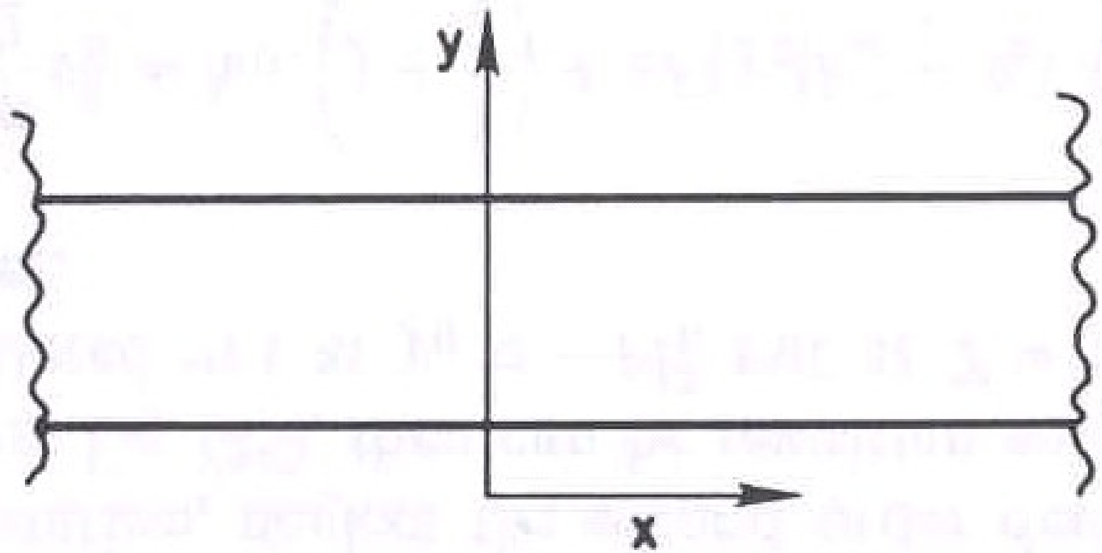
$$f_L(\mu_L) = f(\mu_0) - (df/dE)eV_L + .. \qquad V = V_L - V_R \quad \Longrightarrow$$

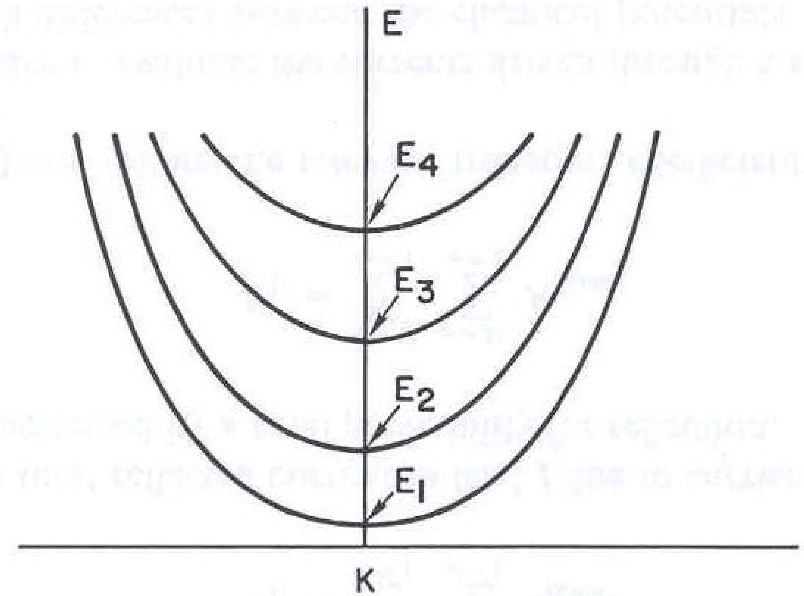
conductance

Transmission probability evaluated in the equilibrium potential

$$G = I/V = \frac{e^2}{h} \int dE\, T(E)\, (-df(E)/dE)$$

Multi-probe conductance: leads





asymptotic perfect translation invariant potential

$$V(x,y) = V(y)$$

separable wave function

$$\phi^{\pm}_{\alpha n}(\mathbf{r}, E) = e^{\pm i k_n(E) x}\, \chi_{\alpha n}(y)$$

energy of transverse motion E_n channel threshold

energy for transverse and longitudinal motion

$$E = E_n + \hbar^2 k^2 / 2m \qquad \Leftrightarrow$$

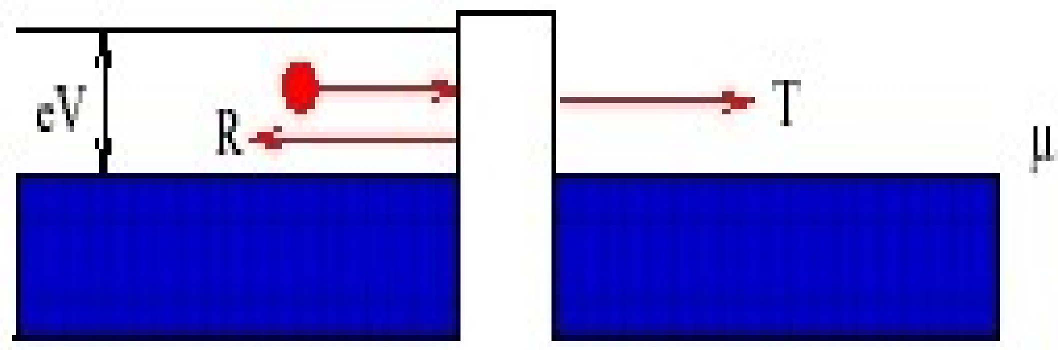
scattering channel

Occupation number and current amplitudes

Buttiker, PRB 46, 12485 (1992)

Incident current at kT = 0

$$I_{in} = (e/h)eV$$



Incident current at kT > 0

$$dI_{in} = (e/h)\, f(E)\, dE$$

Occupation number

$$f(E) = \langle\, n(E)\, \rangle$$

< > = statistical average

Creation and annihilation operators

$$\langle\, \hat{a}^{\dagger}(E)\hat{a}(E')\, \rangle = f(E)\delta(E - E')$$

«Incident current » « Current amplitude » $\hat{a}(E)$

$$\hat{I}_{in}(t) = (e/h) \int dE \int dE'\ \hat{a}^{\dagger}(E)\, \hat{a}(E')\, e^{i(E-E')t/\hbar}$$

$$\hat{I}_{in}(t) = (e/h) \int dE\ \hat{n}(E,t)$$

Current operator

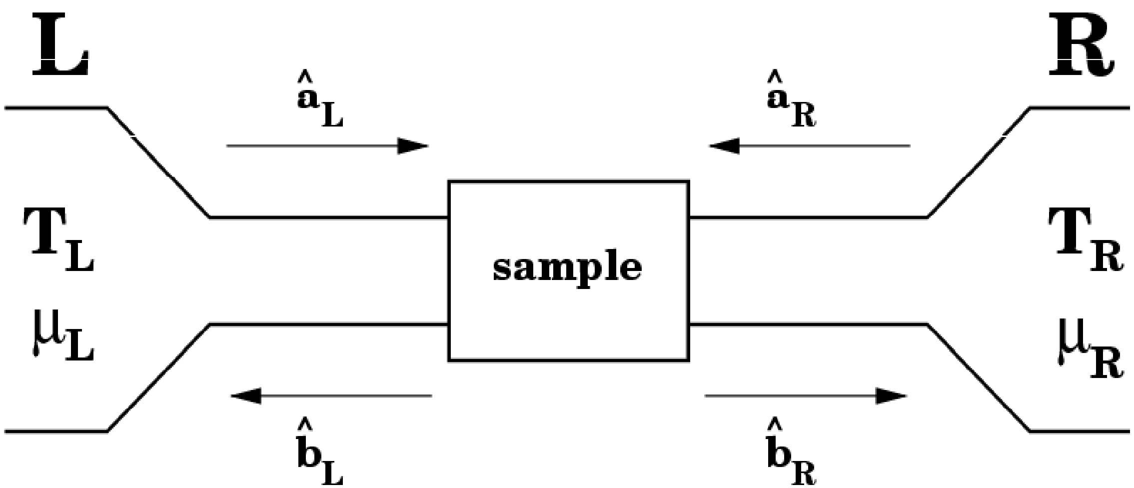
Buttiker, PRL 65, 2901 (1990)

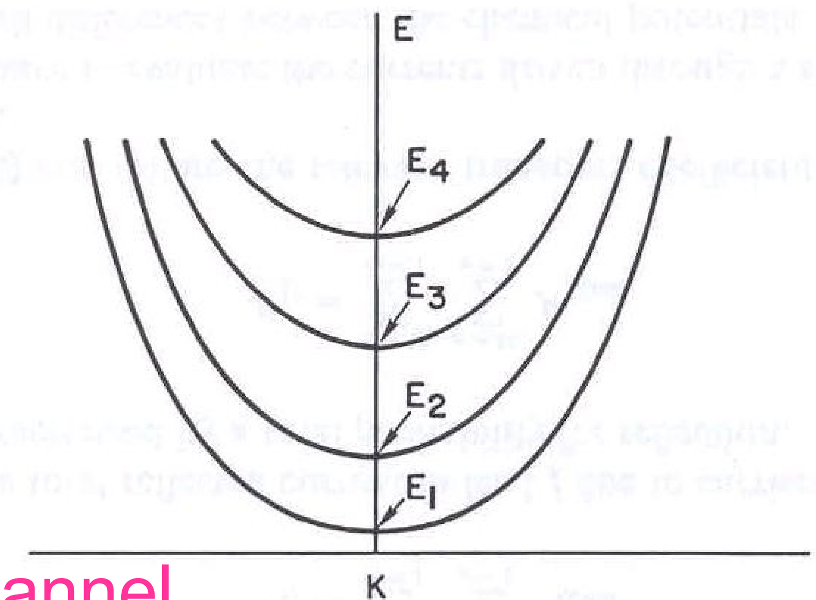
Current in contact α single channel result

$$\hat{I}_\alpha(t) = \frac{e}{h}\int dE\,[\hat{n}_{\alpha,in}(E,t) - \hat{n}_{\alpha,out}(E,t)]$$

current amplitude: $\hat{a}_\alpha(E)$ (incoming) $\hat{b}_\alpha(E)$ (outgoing)

$$\hat{I}_\alpha(t) = \frac{e}{h}\int dE' dE[\hat{a}^\dagger_\alpha(E')\hat{a}_\alpha(E) - \hat{b}^\dagger_\alpha(E')\hat{b}_\alpha(E)]e^{i(E'-E)t/\hbar}$$





Current in contact α multi-channel channel

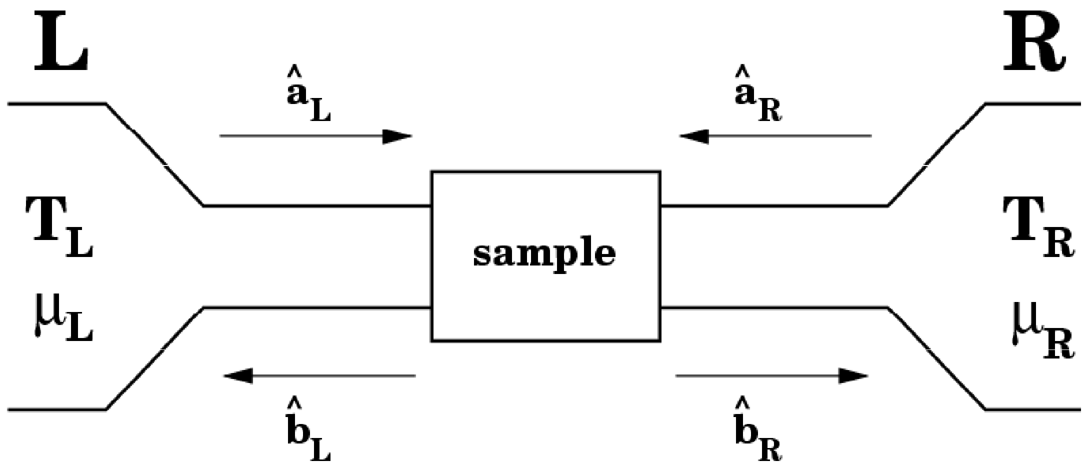
$$\hat{I}_\alpha(t) = \frac{e}{h}\sum_n\int dE' dE[\hat{a}^\dagger_{\alpha n}(E')\hat{a}_{\alpha n}(E) - \hat{b}^\dagger_{\alpha n}(E')\hat{b}_{\alpha n}(E)]e^{i(E'-E)t/\hbar}$$

Current operator

Buttiker, PRL 65, 2901 (1990)

$\hat{a}_\alpha(E)\,,\hat{b}_\alpha(E)\;:\;\; N_\alpha$ component vectors

$$\hat{I}_\alpha(t) = \frac{e}{h}\int dE'\,dE\,[\hat{a}^\dagger_{\alpha n}(E')\hat{a}_\alpha(E) - \hat{b}^\dagger_\alpha(E')\hat{b}_\alpha(E)]e^{i(E'-E)t/\hbar}$$



$$\mathbf{b}_\alpha = \sum_\beta \mathbf{s}_{\alpha\beta}\mathbf{a}_\beta$$

$$\hat{I}_\alpha(t) = \frac{e}{h}\int dE' dE \sum_{\beta,\gamma} \hat{a}^\dagger_\beta(E') A_{\beta\gamma}(\alpha, E', E)\hat{a}_\gamma(E) e^{i(E'-E)t/\hbar}$$

$$A_{\beta\gamma}(\alpha, E', E) = 1_\alpha \delta_{\alpha\beta}\delta_{\alpha\gamma} - s^\dagger_{\alpha\beta}(E') s_{\alpha\gamma}(E)$$

quantum statistical average

$$\langle\, \hat{a}^\dagger_\beta(E)\hat{a}_\gamma(E')\,\rangle = \delta_{\beta\gamma}\,\delta(E-E')\,f_\beta(E) \;\Longrightarrow$$

average current, conductance

Conductance: finite temperature

$$\hat{I}_\alpha(t) = \frac{e}{h}\int dE' dE \sum_{\beta,\gamma} \hat{a}^\dagger_\beta(E') A_{\beta\gamma}(\alpha, E', E)\hat{a}_\gamma(E) e^{i(E'-E)t/\hbar}$$

$$A_{\beta\gamma}(\alpha, E', E) = 1_\alpha \delta_{\alpha\beta}\delta_{\alpha\gamma} - s^\dagger_{\alpha\beta}(E') s_{\alpha\gamma}(E)$$

quantum statistical average

$$\langle \hat{a}^\dagger_\beta(E)\hat{a}_\gamma(E') \rangle = \delta_{\beta\gamma}\, \delta(E - E')\, f_\beta(E) \quad \Longrightarrow$$

$$I_\alpha = \frac{e}{h}\int dE \left[(N_\alpha - R_{\alpha\alpha}) f_\alpha - \sum_{\beta \neq \alpha} T_{\alpha\beta} f_\beta \right]$$

$$R_{\alpha\alpha} = Tr(s^\dagger_{\alpha\alpha} s_{\alpha\alpha}) \qquad T_{\alpha\beta} = Tr(s^\dagger_{\alpha\beta} s_{\alpha\beta})$$

$$f_\alpha(\mu_\alpha) = f(\mu_0) - (df/dE) e V_\alpha + .. \quad \Longrightarrow$$

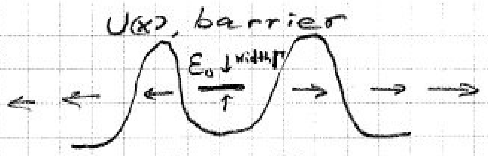
$$I_\alpha = \frac{e}{h}\sum_\beta G_{\alpha\beta} V_\beta \qquad \sum_\alpha G_{\alpha\beta} = 0 \qquad \sum_\beta G_{\alpha\beta} = 0$$

$$G_{\alpha\alpha} = \frac{e^2}{h}\int dE(-df/dE)(N_\alpha - R_{\alpha\alpha})\,; \quad G_{\alpha\beta} = -\frac{e^2}{h}\int dE(-df/dE) T_{\alpha\beta}$$

Advanced Quantum Mechanics: Resonance Scattering

Quasi-bound states

Seek solution of SE



$$\varepsilon\psi = -\frac{\hbar^2}{2m}\psi'' + U(x)\psi$$

with only outgoing wave at infinity, no incoming wave

Tunneling, finite lifetime

⇒ unitarity violated, complex-valued ε

$$\varepsilon = \varepsilon_0 - i\frac{\Gamma}{2} \leftarrow \text{decay rate}$$

Time evolution: $\psi(t) \propto e^{-i\varepsilon t} = e^{-i\varepsilon_0 t}e^{-\frac{1}{2}\Gamma t}$

Ex. SE on semiaxis $x > 0$, $\psi(x=0) = 0$ (hard wall)

$$U(x) = \alpha\,\delta(x - x_0)$$

$$0 < x < x_0 \quad \psi(x) = \frac{\sin kx}{\sin kx_0} \quad (\text{continuity of } \psi \text{ at } x = x_0)$$

$$x_0 < x \quad \psi(x) = e^{ik(x-x_0)} \quad k^2 = 2m\varepsilon/\hbar^2$$

$$\psi'(x_0+) - \psi'(x_0-) = \frac{2m\alpha}{\hbar^2}\psi(x_0) \quad (\text{matching condition})$$

w.f. value

$$ik - k\frac{\cos kx_0}{\sin kx_0} = \frac{2m\alpha}{\hbar^2}$$

$$\sin kx_0 + \frac{k\hbar^2}{2m\alpha}e^{-ikx_0} = 0$$

$$e^{ikx_0} - e^{-ikx_0} - \frac{ik\hbar^2}{m\alpha}e^{-ikx_0} = 0$$

$$e^{2ikx_0} = 1 + \frac{ik\hbar^2}{m\alpha} \leftarrow \text{small correction}$$

Weak tunneling, large α ⇒ $k = \frac{\pi n}{x_0} + \Delta k$

$$\Delta k = \frac{\ln\left(1 + \frac{ik_n\hbar^2}{m\alpha}\right)}{2ix_0} = \Delta k' - i\Delta k'', \quad \Delta k'' = \frac{k_n^2\hbar^4}{4x_0 m^2\alpha^2}$$

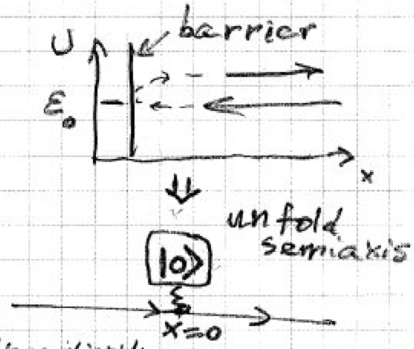
$$\Gamma = 2\,\mathrm{Im}\,\varepsilon = 2\frac{\hbar^2}{m}k_n\Delta k'' = \frac{k_n^3\hbar^6}{2x_0 m^3\alpha^2} = \frac{2\varepsilon_0^2}{\pi n}\frac{\hbar^2}{m\alpha^2}$$

$\hbar p_n$

Resonant scattering

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x)$$

$\Gamma \ll \varepsilon_F$



$$H_{res} = -i\hbar v\frac{d}{dx} + \varepsilon_0|0\rangle\langle 0|$$

$$\lambda\,|x{=}0\rangle\langle 0| + \lambda^*|0\rangle\langle x{=}0|$$

State: $\sum_x \psi(x)|x\rangle + \phi|0\rangle$

$$\varepsilon\psi(x) = -i\hbar v\,\psi'(x) + \lambda\delta(x)\phi$$

discontinuity: $\psi_{x=0-} \neq \psi_{x=0+}$

$$\varepsilon\phi = \varepsilon_0\phi + \lambda^*\int \delta(x)\psi(x)\,dx$$

$$(\langle x|x{=}0\rangle = \delta(x))$$

Understood as

$$(\varepsilon - \varepsilon_0)\phi = \frac{\lambda}{2}\left(\psi(0-) + \psi(0+)\right)$$

Solved by:

$$-i\hbar v\left(\psi(0+) - \psi(0-)\right) + \frac{|\lambda|^2}{2}\frac{\left(\psi(0+) + \psi(0-)\right)}{\varepsilon - \varepsilon_0} = 0$$

$$\psi(0+)\left(\frac{|\lambda|^2}{2(\varepsilon - \varepsilon_0)} - i\hbar v\right) + \psi(0-)\left(\frac{|\lambda|^2}{2(\varepsilon - \varepsilon_0)} + i\hbar v\right) = 0$$

$$\psi(0+)\left(\frac{\Gamma}{2} - i(\varepsilon - \varepsilon_0)\right) + \psi(0-)\left(\frac{\Gamma}{2} + i(\varepsilon - \varepsilon_0)\right) = 0$$

$$\psi(0+) = \psi(0-)\frac{\varepsilon - \varepsilon_0 - i\frac{\Gamma}{2}}{\varepsilon - \varepsilon_0 + i\frac{\Gamma}{2}} \qquad \Gamma = \frac{|\lambda|^2}{\hbar v}$$

Scattering state:

$$\psi(x) = \begin{cases} e^{ikx}, & x < 0 \\ \frac{\varepsilon - \varepsilon_0 - i\Gamma/2}{\varepsilon - \varepsilon_0 + i\Gamma/2}e^{ikx}, & x > 0 \end{cases} \qquad e^{2i\theta} = \frac{\varepsilon - \varepsilon_0 - i\Gamma/2}{\varepsilon - \varepsilon_0 + i\Gamma/2}$$

$$-\cot\theta = 2(\varepsilon - \varepsilon_0)/\Gamma$$

$\theta(\varepsilon)$ changes by π across res

Lifetime of a resonance state

To describe decay,
seek for a state with $\psi_{in} = 0$

$$(\mathcal{E} - \mathcal{E}_0)\phi = \frac{\lambda}{2}(\psi(0+) + 0)$$

$$-i\hbar v(\psi(0+) - 0) + \lambda\phi$$

Solved by: $\frac{|\lambda|^2}{2(\mathcal{E} - \mathcal{E}_0)} = i\hbar v$

Complex energy $\mathcal{E} = \mathcal{E}_0 - i\Gamma/2$

Time evolution:

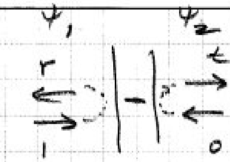
$$\phi(t) \propto e^{-\frac{i}{\hbar}\mathcal{E}t} = e^{-\frac{i}{\hbar}\mathcal{E}_0 t}\, e^{-\frac{\Gamma}{2\hbar}t}$$

$$P(t) = |\phi(t)|^2 \propto e^{-\frac{\Gamma}{\hbar}t} \quad \text{exp. decay}$$

Thus $\tau = \hbar/\Gamma$ is lifetime

Resonance coupled to two leads

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x)$$



↓ unfold semiaxes:

$$H = -i\hbar v\frac{d}{dx_1} - i\hbar v\frac{d}{dx_2} + \mathcal{E}_0|0\rangle\langle 0|$$

$$+ (\lambda_1|x_1=0\rangle + \lambda_2|x_2=0\rangle)\langle 0| + h.c.$$

$\langle x|x_{1,2}=0\rangle = \delta(x)$

Let $\lambda_1 = \lambda_2$, Define $\psi_\pm = \frac{1}{\sqrt{2}}(\psi_1 \pm \psi_2)$ even/odd states

The resonant level couples to ψ_+ only

$$\psi_{+\,out} = e^{2i\theta}\psi_{+\,in}$$

$$\psi_{-\,out} = \psi_{-\,in}$$

$$H = -i\hbar v\frac{d}{dx_+} - i\hbar v\frac{d}{dx_-} + \mathcal{E}_0|0\rangle\langle 0| + \sqrt{2}\lambda\,\delta(x_+)\langle 0| + h.c.$$

Note: $\lambda \to \sqrt{2}\lambda$

$$r + t = e^{2i\theta}$$

$$r - t = 1$$

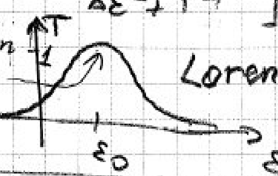
$$r = \frac{1 + e^{2i\theta}}{2} \qquad t = \frac{e^{2i\theta} - 1}{2}$$

$$|r|^2 + |t|^2 = \frac{1}{4}\times 4 + 2\cos 2\theta - 2\cos 2\theta = 1 \quad \text{(Unitarity)}$$

Find transmission $T(\varepsilon) = \frac{1 - \cos 2\theta}{2}$

$$T(\varepsilon) = \frac{1}{4}\left[2 - \frac{\Delta\mathcal{E} - i\Gamma}{\Delta\mathcal{E} + i\Gamma} - c.c.\right] = \frac{1}{4}\left[2 - \frac{2\Delta\mathcal{E}^2 - 2\Gamma^2}{\Delta\mathcal{E}^2 + \Gamma^2}\right]$$

$$= \frac{\Gamma^2}{(\mathcal{E} - \mathcal{E}_0)^2 + \Gamma^2}, \quad T_{max} = 1$$



For non-equal couplings $\lambda_1 \neq \lambda_2$: $\Gamma \to \frac{1}{2}(\Gamma_1 + \Gamma_2)$, Lorentzian, $T_{max} < 1$

?