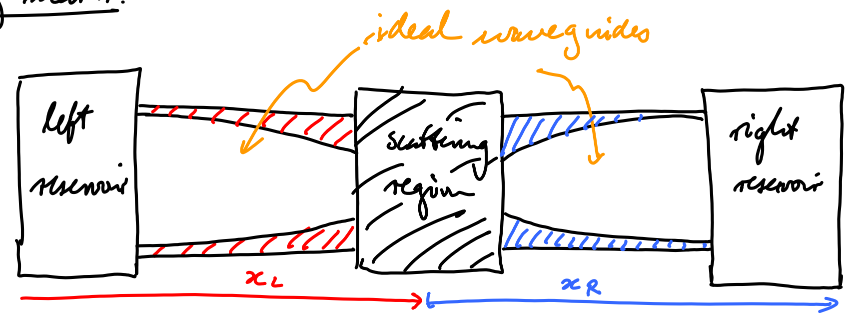
1.3.1 Scattering Matrix (SM)

26.4.2010

General idea: though nanostructures are complex objects depending on many microscopic details, their properties can be characterized in terms of a limited number of parameters: the elements of the scattering matrix.



incident from left: $1 \longrightarrow$, $r \longleftarrow$ $\quad$ $\longrightarrow t$

incident from right: $t' \longleftarrow$ $\quad$ $\longleftarrow 1$, $\longrightarrow r'$

SM2

Wave-functions in left/right wave guides can be described in terms of plane waves,

$$\Psi(x_L, y_L, z_L) = \sum_n \frac{1}{\sqrt{2\pi\hbar v_n}} \Phi_n(y_L, z_L)\left[a_{Ln} e^{ik_x^{(n)} x_L} + b_{Ln} e^{-ik_x^{(n)} x_L}\right] \quad (1)$$

$$\Psi(x_R, y_R, z_R) = \sum_m \frac{1}{\sqrt{2\pi\hbar v_m}} \Phi_m(y_R, z_R)\left[a_{Rm} e^{-ik_x^{(m)} x_R} + b_R e^{+ik_x^{(m)} x_R}\right] \quad (2)$$

with coordinates $x_L < 0$, y_L, z_L / $x_R > 0$, y_R, z_R, mode #: n / m, mode energy E_n / E_m

wave number $k_x^{(n)} = \sqrt{2m(E - E_n)}/\hbar$, likewise for $k_x^{(m)}$. (3)

a: incoming, b: outgoing (reflected or transmitted)

prefactor $\frac{1}{\sqrt{v}}$: to ensure that current $\psi^{+}\psi v$ is independent of v and depends only on a, b.

Solving SE will yield linear relation among coefficients: **(SM3)**

$$b_{\alpha l} = \sum_{\alpha'=L,R} \sum_{l'=1}^{N_{\alpha'}} S_{\alpha l,\alpha' l'} \, a_{\alpha' l'} \qquad \begin{array}{l} \alpha = L,\ l = 1,\dots,N_L \\ \alpha = R,\ l = 1,\dots,N_R \end{array} \tag{1}$$

$\uparrow$ outgoing $\quad N_L \leftarrow \boxed{\ } \rightarrow N_R$ $\qquad\qquad$ $\uparrow$ incoming $\quad N_L \rightarrow \boxed{\ } \leftarrow N_R$

combined indices (α, l) and (α', l') take on $N_L + N_R$ values:

$S_{\alpha l,\alpha' l'}$ is $(N_L + N_R) \times (N_L + N_R)$ - dimensional matrix

Block structure:

$$\hat{S} = \begin{array}{cc} N_L \times N_L & N_L \times N_R \\ \left(\begin{array}{cc} \hat{S}_{LL} & \hat{S}_{LR} \\ \hat{S}_{RL} & \hat{S}_{RR} \end{array}\right) & \\ N_R \times N_L & N_L \times N_L \end{array} \equiv \begin{pmatrix} \hat{r} & \hat{t}' \\ \hat{t} & \hat{r}' \end{pmatrix} \tag{2}$$

(SM4)

reflection matrices $\quad \hat{r} : N_L \times N_L$ describes $L \to L$ scattering
$\qquad\qquad\qquad\quad\ \hat{r}' : N_R \times N_R \qquad\quad R \to R$

transmission matrices: $\hat{t} : N_R \times N_L \qquad L \to R$ $\qquad$ (1)
$\qquad\qquad\qquad\qquad\quad\ \hat{t}' : N_L \times N_R \qquad L \to R$

E.g. probability for $L,n \to L,n'$ scattering is $|r_{nn'}|^2$, etc.

Total probability for electron in channel L,n to be reflected or transmitted:

$$R_n = \sum_{n'} |r_{n'n}|^2 = (\hat{r}^\dagger \hat{r})_{nn} \; ; \qquad T_n = \sum_m |t_{mn}|^2 = (t^\dagger t)_{nn} \tag{2}$$

$$R_m = \sum_{m'} |r'_{m'm}|^2 = (\hat{r}'^\dagger \hat{r}')_{mm} \; ; \qquad T_m = \sum_n |t'_{nm}|^2 = (t'^\dagger t')_{mm} \tag{2'}$$

Each electron is either reflected or transmitted:

$$1 = R_n + T_n = (s^\dagger s)_{nn} \tag{3}$$

$$1 = R_m + T_m = (s^\dagger s)_{mm} \tag{3'}$$

These are special cases of a general statement in QM:

SM5

$\hat{S}$-matrix is unitary: $\hat{S}^\dagger . \hat{S} = \hat{1}$ and $\hat{S}.\hat{S}^\dagger = 1$ (1)

This implies that $\hat{t}\hat{t}^\dagger$, $\hat{t}^\dagger\hat{t}$, $\hat{t}'\hat{t}'^\dagger$, $\hat{t}'^\dagger\hat{t}'$ have same nonzero eigenvalues $\{T_p\}$

$\hat{r}\hat{r}^\dagger$, $\hat{r}^\dagger\hat{r}$, $\hat{r}'\hat{r}'^\dagger$, $\hat{r}'^\dagger\hat{r}'$ " " nonunity " $\{R_p\} = \{1-T_p\}$

Proof:

$$\begin{pmatrix} \hat{r}^\dagger & \hat{t}^\dagger \\ \hat{t}'^\dagger & \hat{r}'^\dagger \end{pmatrix}\begin{pmatrix} \hat{r} & \hat{t}' \\ \hat{t} & \hat{r}' \end{pmatrix} \overset{(3.2)\,(1)}{=} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \hat{r} & \hat{t}' \\ \hat{t} & \hat{r}' \end{pmatrix}\begin{pmatrix} \hat{r}^\dagger & \hat{t}^\dagger \\ \hat{t}'^\dagger & \hat{r}'^\dagger \end{pmatrix} \overset{(3.2)\,(1)}{=} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad (2)$$

$\hat{r}^\dagger\hat{r} + \hat{t}^\dagger\hat{t} = 1$ (3) $\qquad \hat{r}\hat{r}^\dagger + \hat{t}'\hat{t}'^\dagger = 1$ (3')

$\hat{r}^\dagger\hat{t}' + \hat{t}^\dagger\hat{r}' = 0$ (4) $\qquad \hat{r}\hat{t}^\dagger + \hat{t}'\hat{r}'^\dagger = 0$ (4')

$\hat{t}'^\dagger\hat{r} + \hat{r}'^\dagger\hat{t} = 0$ (5) $= (4)^\dagger$ $\qquad \hat{t}\hat{r}^\dagger + \hat{r}'\hat{t}'^\dagger = 0$ (5') $= (4')^\dagger$

$\hat{t}'^\dagger\hat{t}' + \hat{r}'^\dagger\hat{r}' = 1$ (6) $\qquad \hat{t}\hat{t}^\dagger + \hat{r}'\hat{r}'^\dagger = 1$ (6')

SM6

Now:

$\hat{t}' \overset{(5.4')}{=} -\hat{r}\hat{t}^\dagger(\hat{r}'^\dagger)^{-1}$ (1) $\qquad \hat{t}'^\dagger \overset{(5.5)}{=} -\hat{r}'^\dagger\hat{t}\,\hat{r}^{-1}$ (1')

(7)(7'): $\hat{t}'\hat{t}'^\dagger = \hat{r}\hat{t}^\dagger\hat{t}\hat{r}^{-1}$ (2)

Similarly: $\hat{t}'^\dagger \overset{(5.5')}{=} (\hat{r}')^{-1}\hat{t}\hat{r}^\dagger$ (3) $\qquad \hat{t}' \overset{(5.4)}{=} (\hat{r}^\dagger)^{-1}\hat{t}^\dagger\hat{r}'$ (3)

(9)(9'): $\hat{t}'^\dagger\hat{t}' = (\hat{r}')^{-1}\hat{t}\hat{t}^\dagger\hat{r}'$ (4)

"transmission eigenvalues"

Let $\hat{t}\hat{t}^\dagger$ have the set of eigenvalues $\{T_p\}$. (5)

Then $\det(\hat{t}\hat{t}^\dagger - T_p) = 0 \;\; \forall$ eigenvalue T_p. (6)

SM7

The same is true for :

$$\det\left(\hat{t}^{\dagger}\hat{t} - T_p\right) \overset{(6.5)}{=} 0 \qquad \text{(from cyclic invariance of trace)} \qquad (1)$$

$$\det\left(\hat{t}'^{\dagger}\hat{t}' - T_p\right) \overset{(6.4)}{=} 0 \qquad \text{since } \det\left(A\,B\,A^{-1}\right) = \det B \qquad (2)$$

$$\det\left(\hat{t}'\hat{t}'^{\dagger} - T_p\right) \overset{(6.2)}{=} 0 \qquad \text{" \quad " \quad "} \qquad (3)$$

So: $\boxed{\underbrace{\hat{t}\hat{t}^{\dagger},\ \hat{t}'^{\dagger}\hat{t}'}_{N_L \times N_L},\ \underbrace{\hat{t}^{\dagger}\hat{t},\ \hat{t}'\hat{t}'^{\dagger}}_{N_R \times N_R} \ \text{all have same non-zero eigenvalues } \{T_p\}}$ (4)

$\hat{t}$ and $\hat{t}'^{\dagger}$ are $N_R \times N_L$, $\hat{t}^{\dagger}$ and $\hat{t}'$ are $N_L \times N_R$

SM8

From (5.3)

$$\hat{t}^{\dagger}\hat{t} = -\hat{r}^{\dagger}\hat{r} + 1$$

$$\Rightarrow \quad 0 \overset{(7.1)}{=} \mathrm{Tr}\left(t^{\dagger}t - T_p\right) = -\mathrm{tr}\left(\hat{r}^{\dagger}\hat{r} - 1 + T_p\right)$$

so, if $T_p \neq 0$, then $R_p = 1 - T_p \neq 1$ is eigenvalue of $\hat{r}^{\dagger}\hat{r}$

similarly, the same is true for

So: $\boxed{\hat{r}^{\dagger}\hat{r},\ \hat{r}\hat{r}^{\dagger},\ \hat{r}'\hat{r}'^{\dagger},\ \hat{r}'^{\dagger}\hat{r}' \ \text{all have same set of eigenvalues } \{R_p\} \text{ different from } 1, \text{ with } R_p = 1 - T_p}$

SM9

<u>Time-reversal symmetry:</u>

if this symmetry holds, S-matrix is symmetric: $\hat{S} = \hat{S}^T$ (1)

Intuitively: $b = \hat{S} a$ (in → out scattering) (2)

$(1)^*$ $b^* = \hat{S}^* a = \underbrace{(\hat{S}^+)^T}_{\hat{S}^+ \text{ if (1) holds}} a = \hat{S}^+ a$ (3)

$\hat{S}\,(3)$: $\hat{S} b^* = a^* \Rightarrow$ (out → in scattering) (4)

So, $\hat{S}$ describes both in → out and out → in scattering, as expected for time-reversal symmetry.

$\hat{S} = \hat{S}^T \Rightarrow \hat{r} = \hat{r}^T$ and $\hat{t}' = \hat{t}^T$ (5)

SM10

In presence of magnetic field: $\vec{B} \xrightarrow{\text{time-reversal}} -\vec{B}$ (1)

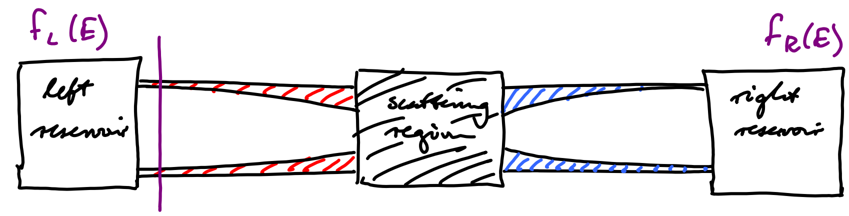
So: $\hat{S}(B) = \hat{S}^T(-B)$ (2)

$\hat{r}(B) = \hat{r}^T(-B)$, $\hat{r}'(B) = \hat{r}'^T(-B)$ (3)

$\hat{t}(B) = \hat{t}'(-B)$ (4)

SM11

1.3.2 Transmission Eigenvalues



current at $x_L = -\infty$:

$$\text{(Intro 15.3)} \quad I = 2_s e \sum_n \int_{-\infty}^{\infty} \frac{dk_x}{2\pi} v_x(k_x) f_n(k_x) \tag{1}$$

	came from	with probability	$f_n(k_x)$	
$k_x > 0$	left	1	$f_L(E)$	(2)
$k_x < 0$	left	$R_n(E) = \sum_{n'} \lvert r_{n'n}\rvert^2 \overset{(4.3)}{=} 1 - T_n(E)$	$f_L(E)$	(3)
$k_x < 0$	right	$T_n(E) = \sum_m \lvert t_{nm}\rvert^2 \overset{(4.2)}{=} (t^\dagger t)_{nn}$	$f_R(E)$	(4)

SM12

$$I \overset{(11.1)}{=} 2_s e \sum_n \int_0^\infty \frac{dk_x}{2\pi} v_x(k_x) \underbrace{\left[\cancel{f_L(E)} \overset{(11.2)}{-} (\cancel{1} - T_n(E)) f_L(E) - T_n(E) f_R(E) \right]}_{[f_L(E) - f_R(E)]\, T_n(E)} \tag{1}$$

$$T_n(E) = (t^\dagger t)_{nn}$$

Change variables: $$\frac{1}{2\pi}\int dk_x \, v_x(k_x) \overset{\text{(Intro 17.3)}}{=} \frac{1}{h}\int dE \tag{2}$$

$$I = \underbrace{\frac{2_s e^2}{h}}_{G_Q} \int_0^\infty dE \frac{1}{e} \underbrace{\sum_n (t^\dagger t)_{nn}}_{= T_r(t^\dagger t)} \left[f_L(E) - f_R(E) \right] \tag{3}$$

$$= T_r(t^\dagger t) \overset{(17.4)}{=} \sum_p T_p(E) \tag{4}$$

"transmission eigenvalues"

rewrite in eigenbasis of $t^\dagger t$

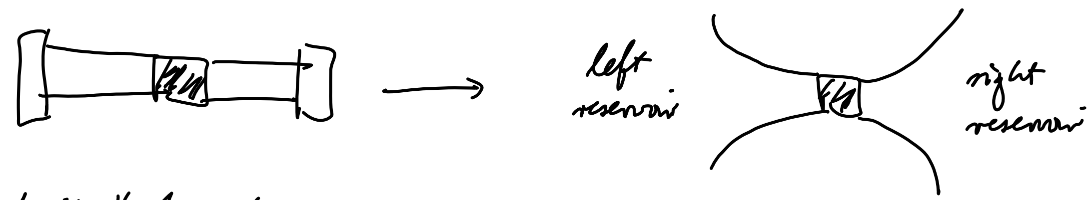
In linear regime, small voltage, $T(E) \simeq T(\mu)$,
$\int dE/e \, (f_L - f_R) = eV$.

$$\Longrightarrow \quad G = \frac{I}{V} = G_Q \sum_p T_p(\mu) \tag{5}$$

"two-terminal Landauer formula"

SM13

- For real nanostructure, "open up waveguides":



finite # of modes N_L, N_R

infinite # of modes, $N_L = \infty$, $N_R = \infty$, but only finite # of $T_p \neq 0$.

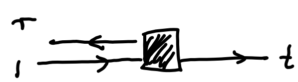
- Determine scattering matrix by solving SE in real geometry, matching solution to asymptotics of (2.1), (2.2).

"Tedious & boring", and results depend on sample-specific details. We need to learn how to distill essential features!

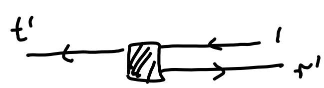
SM14

<u>One channel scatter</u>

incoming from left:



incoming from right:



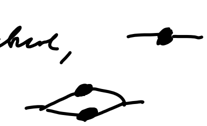
reflection & transmission coefficients: $R = 1 - T$, with

$$R = |r|^2 = |r'|^2 \quad , \quad T = |t|^2 = |t'|^2$$

unitary $\hat{S}$-matrix can be parametrized by:

$$\hat{S} = \begin{pmatrix} \sqrt{R}\, e^{i\theta} & \sqrt{T}\, e^{i\eta} \\ \sqrt{T}\, e^{i\eta} & -\sqrt{R}\, e^{i(2\eta-\theta)} \end{pmatrix}$$

Phases θ, η do not influence conductance of single structure, but show up in interference effects for two structures.



Check: does this satisfy Eqs. (5.3) − (5.6) ?

SM15

$$\hat{r}^\dagger \hat{r} + \hat{t}^\dagger \hat{t} = 1 \qquad R + T = 1 \quad ✓$$

$$\hat{r}^\dagger \hat{t}' + \hat{t}^\dagger \hat{r}' = 0 \qquad \sqrt{RT}\left(e^{-i\theta} e^{i\eta} - e^{-i\eta} e^{i(2\eta-\theta)}\right) = 0 \quad ✓$$

$$\hat{t}'^\dagger \hat{r} + \hat{r}'^\dagger \hat{t} = 0 \qquad \sqrt{RT}\left(e^{-i\eta} e^{i\theta} - e^{-i(2\eta-\theta)} e^{i\eta}\right) = 0 \quad ✓$$

$$\hat{t}'^\dagger \hat{t}' + \hat{r}'^\dagger \hat{r}' = 1 \qquad T + R = 0 \quad ✓$$

$$\hat{r}\hat{r}^\dagger + \hat{t}'\hat{t}'^\dagger = 1 \qquad R + T = 1 \quad ✓$$

$$\hat{r}\hat{t}^\dagger + \hat{t}'\hat{r}'^\dagger = 0 \qquad \sqrt{RT}\left(e^{i(\theta-\eta)} - e^{i\eta-(2\eta-\theta)}\right) = 0 \quad ✓$$

$$\hat{t}\hat{r}^\dagger + \hat{r}'\hat{t}'^\dagger = 0 \qquad \sqrt{RT}\left(e^{i(\eta-\theta)} - e^{i(2\eta-\theta)-i\eta}\right) = 0$$

$$\hat{t}\hat{t}^\dagger + \hat{r}'\hat{r}'^\dagger = 1 \qquad T + R = 1 \quad ✓$$

SM16

For ideal systems (rectangular barrier, adiabatic, symmetric, point contact), there is "no mode mixing", i.e. $N_L = N_R$, and r, t, r', t' and $t^\dagger t$ are diagonal.

So, $$t^\dagger t = \begin{pmatrix} T_1 & & & \\ & T_2 & & \\ & & \ddots & \\ & & & T_N \end{pmatrix},$$ "transmission eigenvalues" are the the actual transmission coefficients of system.

1.3.3 Distribution of Eigenvalues

SM17

T_p are random numbers, depending on sample-specific details.

Design of a nanostructure is characterized by <u>distribution</u> of T_p's.

$$P(T) = \Big\langle \sum_p \delta(T - T_p(E)) \Big\rangle = \begin{cases} \text{smooth function if } \langle G \rangle \gg G_Q \\ \text{spikey function if } \langle G \rangle \simeq G_Q \end{cases}$$

$\langle\ \rangle$ = average over ensemble of many nanostructures of same design (same shape, impurity concentration, etc.)

$$\frac{\#\text{ of } T_p\text{'s between } T \text{ and } T + dT}{\#\text{ of nanostructures}} \equiv T(P)\,dT$$

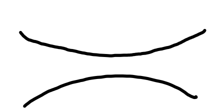
Ensemble average of an arbitrary function of the T's:

$$\Big\langle \sum_p f(T_p) \Big\rangle = \Big\langle \int_0^1 dT \sum_p \delta(T - T_p)\, f(T) \Big\rangle = \int_0^1 dT\, P(T) f(T)$$

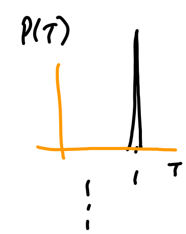
Example 1:

SM18

Clean QPC with N_{open} open channels $(T = 1)$
∞ closed channels $(T = 0)$



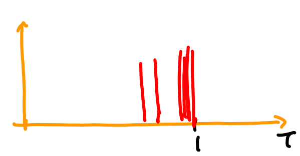
$$P(T) = N_{open}\, \delta(1 - T) + \underbrace{\infty\, \delta(T)}_{\text{can be dropped for transport calculations}}.$$



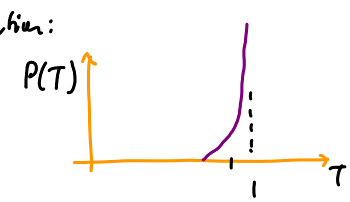
$$P_{clean\text{-}QPC}(T) = N_{open}\, \delta(1 - T)$$

Disorder causes mixing of channels and lifts degeneracy of tr. eigenvalues:

concrete realization

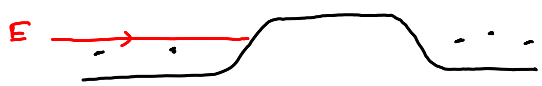


distribution:



SM19

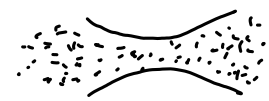
Example 2: wide barrier + defects:



$P(T) =$ 

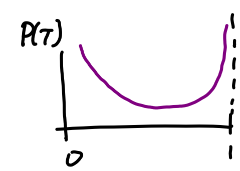
most T_p are near 0, but some are larger (giving tail of distr.), since electrons reflected off barrier can be reflected back toward barrier and "try again"

Example 3: QPC + very many defects:



if $N_{open} \gg 1$, motion is diffusive, presence of QPC becomes irrelevant. Then it can be shown that

$$P_{\text{Diffusive}} = \frac{\langle g \rangle}{2 g_Q} \frac{1}{T\sqrt{1-T}} \qquad (1)$$



Total number of transport channels: $N = \int_0^1 dT\, P(T)\, T$

For (1), $N = \infty$, since infinitely many channels contribute to diffusive transport.