

## Mesoscopic Physics

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## Sheet 9

**1. Combination of S-matrices and the double- $\delta$  potential**

Consider a quasi-1D wire (only 1 propagating mode) with two identical scatterers at  $x = 0$  and  $x = d$  respectively. The scattering potential is approximated by

$$U(x) = U_0 [\delta(x) + \delta(x - d)] . \quad (1)$$

- (a) Show that the transmission and reflection probabilities are given by

$$T_1 = \frac{\hbar^2 v^2}{\hbar^2 v^2 + U_0^2} \quad R_1 = \frac{U_0^2}{\hbar^2 v^2 + U_0^2} \quad (2)$$

with the velocity  $v = \sqrt{2E/m}$ .

(*Hint:* Remember the special matching conditions for the wavefunctions at a  $\delta$ -like potential from QM I.)

- (b) Use the procedure of coherent S-matrix combination to show that the total transmission probability is given by

$$T = T(E) = \frac{T_1^2}{1 - 2R_1 \cos(\theta) + R_1^2} \quad (3)$$

with  $\theta = 2 [dmv/\hbar + \tan^{-1}(\hbar v/U_0)]$  and plot  $T(E)$  for  $U_0 = 9 \text{ eV } \text{\AA}$ ,  $d = 50 \text{ \AA}$  and  $0 < E < 250 \text{ meV}$ .

- (c) • Resonant transmission: Although the individual transmission probability  $T_1$  is usually very small,  $T$  can become large for certain resonant energies. What is the maximum value for  $T$ ? For strong scatterers  $U_0 \gg \hbar v$ , calculate the positions of the resonances  $E_n$ .

please turn over

## 2. Transfer matrix formalism and the double barrier potential

While the scattering matrix  $S$  connects incoming and outgoing waves, the *transfer matrix*  $\mathcal{T}$  connects waves on the left side and waves on the right side of a scatterer in a (quasi-)onedimensional problem.



In the schematic notation of the figure, the transfer matrix is defined as

$$\begin{pmatrix} out' \\ in' \end{pmatrix} = \mathcal{T} \begin{pmatrix} in \\ out \end{pmatrix} \quad (4)$$

- (a) • Show that for a scatterer with transmission and reflection amplitudes  $t$  and  $r$  for particles coming from the left and  $t'$  and  $r'$  for particles coming from the right



the transfer matrix is

$$\mathcal{T} = \begin{pmatrix} t - \frac{rr'}{t'} & \frac{r'}{t'} \\ -\frac{r}{t'} & \frac{1}{t'} \end{pmatrix} \quad (5)$$

By convention within the transfer matrix formalism, the waves are normalized to unit probability, not to unit flux as for the scattering matrix. Therefore the Transmission is in general given by

$$T = \frac{v'}{v} |t|^2 = \frac{v}{v'} |t'|^2 = \frac{v}{v'} \frac{1}{|\mathcal{T}_{22}|^2}, \quad (6)$$

where  $v$  and  $v'$  are the velocities on the left and right side respectively.

- (b) • If one has a series of scatterers, how are the individual transfer matrices combined to give the transfer matrix of the full system?  
(c) Consider a rectangular barrier

$$U(x) = \begin{cases} U & a \leq x \leq b \\ 0 & \text{else} \end{cases} \quad (7)$$

and use the transfer matrix formalism to show that the transmission and reflection amplitudes for  $E < U$  are given by

$$t = \frac{e^{ik(b-a)}}{\cosh[\kappa(b-a)] + i\frac{\varepsilon}{2} \sinh[\kappa(b-a)]} \quad r = -i\frac{\eta}{2} \frac{\sinh[\kappa(b-a)] e^{ik(b-a)}}{\cosh[\kappa(b-a)] + i\frac{\varepsilon}{2} \sinh[\kappa(b-a)]} \quad (8)$$

with  $\kappa = \sqrt{2m(U-E)}/\hbar$ ,  $\varepsilon = \kappa/k - k/\kappa$  and  $\eta = \kappa/k + k/\kappa$ . Herefore determine the transfer matrices for the first potential step, the piece within the barrier and the second step and combine them.

- (d) • Now consider two barriers in series with transfer matrices  $\mathcal{T}_1$  and  $\mathcal{T}_2$  and transmission/reflection amplitudes  $t_1, r_1, t_2$  and  $r_2$ .

$$U(x) = \begin{cases} U_1 & 0 \leq x \leq W_1 \\ U_2 & W_1 + d \leq x \leq W_1 + d + W_2 \\ 0 & \text{else} \end{cases} \quad (9)$$

Note that the free space between the barriers also has a transfer matrix  $\mathcal{T}_d$ . Combine the transfer matrices again to show that the total Transmission is given by

$$T = \left| \frac{t_1 t_2}{1 - r_1 r_2 e^{2ikd}} \right|^2 \quad (10)$$

(Hint: Use the relation  $(\mathcal{T}_{1/2})_{11} = (\mathcal{T}_{1/2})_{22}^*$ .

Can you prove by it looking at the time reversed problem  $\psi \rightarrow \psi^*$ ?)

- (e) • Plot  $T$  for identical barriers ( $U_1 = U_2$ ,  $W_1 = W_2$ ) for different parameter sets such that

$$\begin{aligned} d + \frac{1}{2}(W_1 + W_2) &= 50 \text{ \AA} \\ W_1 U_1 &= W_2 U_2 = 9 \text{ eV} \\ U_1, U_2 &< 250 \text{ meV} \\ 0 < E &< 250 \text{ meV}. \end{aligned}$$

Compare with exercise 1.

- (f) Use the method of finite differences and the Fisher-Lee relations to solve the double barrier problem numerically:

- Show that the second derivative of the wavefunction has to be discretized as

$$\begin{aligned} \psi(x) &\rightarrow \psi(x_i) \equiv \psi_i \\ \psi''(x) &\rightarrow \psi''(x_i) = \frac{\psi_{i+1} - 2\psi_i + \psi_{i-1}}{a^2} \end{aligned} \quad (11)$$

with the lattice spacing  $a$ . This leads to the discrete Schrödinger equation  $H_{ij}\psi_j = E\psi_i$  with

$$H_{ij} = (2t + V_i)\delta_{ij} - t\delta_{i+1,j} - t\delta_{i-1,j}. \quad (12)$$

$t = \hbar^2/2ma^2$  is the hopping parameter and  $V_i \equiv V(x_i)$ .

- In the lecture it was shown that the problem of inverting the full (infinite) matrix  $E - H$  can be avoided by using the finite sized Hamiltonian of the scattering region  $H_S$  and taking the leads into account by adding the so-called self energy  $\Sigma^{R/A}$  with

$$\Sigma_{ij}^R = -\delta_{ij} t e^{ika} [\delta_{1j} + \delta_{Nj}] \quad (13)$$

and  $\Sigma_{ij}^A = (\Sigma_{ji}^R)^*$  for identical leads in 1D. “1” and “ $N$ ” are the first and the last point in the scattering region respectively. The retarded/advanced Green function of the scattering region is then

$$G_S^{R/A} = \frac{\hbar}{a} \left( E - H_S - \Sigma^{R/A} \right)^{-1}. \quad (14)$$

Set up  $H_S$  and calculate  $G_S^{R/A}$  numerically. You can use for example Matlab to invert the matrix.

- Relate the Green function to the transmission using the Fisher-Lee relation derived in class

$$T = \text{Tr} [\Gamma G_S^R \Gamma G_S^A] \quad \Gamma = i[\Sigma^R - \Sigma^A]. \quad (15)$$

- Plot the result for different parameters and lattice spacings.

## Frohes Schaffen!