

# Evanescent modes in a multiple scattering factorization

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We discuss differences between the exact S-matrix for scattering on serial structures and a known factorized expression constructed of single-element S-matrices. As an illustration, we use an exactly solvable model of a quantum wire with two point impurities.

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The core of the scattering–operator concept is that it relates asymptotic states far away from the region where the interaction affects the motion substantially. It happens often, however, that the interaction is localized to a certain domain  $\Omega$ ; since solutions to the free equation are usually known, we may rephrase then the scattering problem as a map between the solutions at the boundary of  $\Omega$  which can be continued (in some direction) into the corresponding asymptotic states. If we want to keep a terminological distinction, it is more appropriate to speak about the *prescattering* operator in this case.

Such a “finite–distance” scattering is particularly useful in situations when the interaction support is a union of a finite number of domains  $\Omega_j$ ; it can help to solve the full problem by means of scattering on the “components”. This subject has become actual in connection with recent studies of quantum–wire superlattices [1–13] in which a number of elements, usually of the same type, is arranged into a serial structure. The physically relevant quantity is the conductivity which is related directly to the electron scattering in the superlattice by Landauer’s formula.

There are several ways how to derive the S–matrix components of the serial structure, *i.e.*, transmission and reflection amplitudes from analogous quantities of a single element. The above sketched observation applies directly if the number of linearly independent solutions entering and leaving each component scatterer is finite. This is the case, *e.g.*, when the system in question is a graph [3, 4]; it may not be easy to find the solution interconnecting the scatterers if an external field is applied, but the algebraic part of the problem is well established [14, 15].

However, quantum mechanics lures always around ready to show who is the master of our physical world. In general, different components of the wave function, say, different transverse modes in a quantum wire, do not cease to be correlated even out of the support of the interaction. Here the difference between the scattering and prescattering operator shows, because the sets of states the latter maps onto each other are larger; in addition to true asymptotic states which live eternally they contain also such that die out when the distance from the interaction region increases.

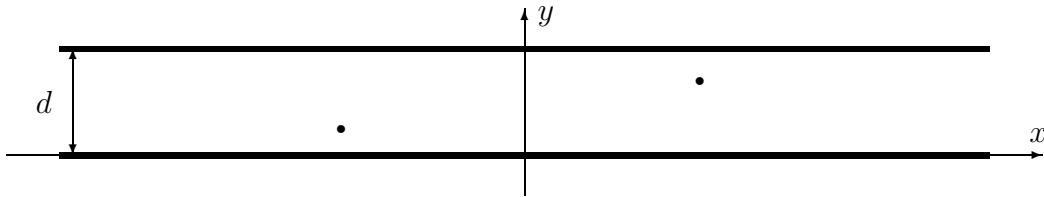


Figure 1: A pair of scatterers in the strip.

It would be certainly worth to formulate properly relations between this approach, which is inherently time-independent, and the rigorous scattering theory [16, 17]. Our aim here, however, is more practical and connected with the mentioned studies of quantum-wire superlattices. With few exceptions their authors include the evanescent states into the iterative procedures of computing the S-matrix, so the result suffers no theoretical defect. The weak point of all numerical calculations stems from the necessity to restrict the used family of states to a finite number; the stability aspect is usually handled by a vague observation that the involved series converge fast enough. In this letter we want to discuss this problem in more detail; we are going to derive explicit error estimates in a solvable model in which the individual scatterers are point impurities in a straight strip.

## 1 S-matrix factorization

Elements of a one-dimensional superlattice are linearly arranged and most authors use various transfer-matrix modifications connecting solutions to the left and right of a given scatterer [1,2,5,9-11]; some admit numerical problems due to a fast growth of higher evanescent modes. It has been argued recently [12] that the approach, which we called pre-S-matrix, offers a more stable scheme relating instead the ingoing and outgoing waves.

Consider therefore a pair of scatterers  $S_1, S_2$  as sketched on Figure 1, where  $A_+$  is the family of solutions entering  $S_1$  from the left *etc.*; in particular, if the corresponding external motion is free,  $A_+$  is

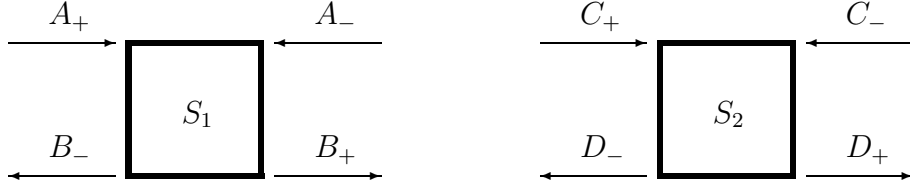


Figure 2: A pair of point scatterers in the strip.

a column vector  $(a_\ell^{(+)} e^{ik_\ell x})$  with  $k_\ell$  being the channel momenta. The pre-S-matrices can be written in terms of the reflection and transmission parts,

$$\begin{pmatrix} B_- \\ B_+ \end{pmatrix} = \begin{pmatrix} R_1 & \tilde{T}_1 \\ T_1 & \tilde{R}_1 \end{pmatrix} \begin{pmatrix} A_+ \\ A_- \end{pmatrix}, \quad \begin{pmatrix} D_- \\ D_+ \end{pmatrix} = \begin{pmatrix} R_2 & \tilde{T}_2 \\ T_2 & \tilde{R}_2 \end{pmatrix} \begin{pmatrix} C_+ \\ C_- \end{pmatrix}, \quad (1)$$

where the tilded quantities corresponding to the passage from the right to the left are obtained from  $R_j, T_j$  by mirror transformation. The above form is convenient because the numbers of involved modes at the two sides of  $S_j$  may be different. Let us stress that the pre-S-matrices in this setting need not be unitary. The evanescent modes — if included — do not contribute to the probability current, and the propagating ones enter with different velocities: if the corresponding part of  $S_j$  should be unitary, we have to multiply the  $(n, m)$ -th amplitudes by  $(k_m/k_n)^{1/2}$ .

Our aim is to express  $B_-, D_+$  from given  $A_+, C_-$ . The relations (1) yield a set of four operator equations which can be solved if we identify the left and right traveling solutions between the scatterers,  $D_- = A_-$  and  $C_+ = B_+$ . Using the identity

$$I + X(I - YX)^{-1}Y = (I - XY)^{-1}$$

which is valid whenever the inverses make sense, we find by a straightforward algebra that the combined pre-S-matrix is

$$S_{12} = \begin{pmatrix} R_1 + \tilde{T}_1(I - R_2\tilde{R}_1)^{-1}R_2T_1 & \tilde{T}_1(I - R_2\tilde{R}_1)^{-1}\tilde{T}_2 \\ T_2(I - \tilde{R}_1R_2)^{-1}T_1 & \tilde{R}_2 + T_2(I - \tilde{R}_1R_2)^{-1}\tilde{R}_1\tilde{T}_2 \end{pmatrix}. \quad (2)$$

The blocks of this operator acquire an illustrative meaning if we expand the inverses into geometric series [6]. Sometimes  $S_2$  is obtained by shifting and/or mirroring another scatterer, then one has to find the operator which represents this transformation. This is equivalent to finding the general solution in the intermediate region between  $S_1$  and  $S_2$  which may not be easy if the motion is not free there [15].

The operator (2) describes the combined scatterer exactly if the space into which  $S_1$  and  $S_2^{-1}$  map is large enough to accommodate all generalized eigenvectors of the corresponding Schrödinger equation. A truncation induces an error which in general is not easy to estimate; we shall do that below in an explicitly solvable model.

## 2 Point–interaction scattering in a strip

The model describes a nonrelativistic particle confined to a straight strip of a width  $d$  with the hard-wall boundary subject to point perturbations simulating natural or artificial impurities. Such a system has numerous interesting features which will be described in detail elsewhere [18]; here we restrict ourselves to a basic information.

For simplicity we set  $d := \pi$  and  $\hbar^2/2m = 1$ , so that in the absence of the impurities the motion is governed by the Hamiltonian  $H_0 := -\Delta$ ; the wavefunction is supposed to satisfy the Dirichlet boundary conditions  $\psi(x, 0) = \psi(x, \pi) = 0$  for any  $x$ . Point interactions situated at  $\vec{a}_j = (a_j, b_j)$ ,  $j = 1, \dots, J$  can be introduced in the standard way [19, Sec.I.5]: they are determined by the boundary conditions

$$L_1(\psi, \vec{a}_j) + 2\pi\alpha_j L_0(\psi, \vec{a}_j) = 0, \quad j = 1, \dots, J,$$

relating the generalized boundary values

$$L_0(\psi, \vec{a}) := \lim_{|\vec{x}-\vec{a}| \rightarrow 0} \frac{\psi(\vec{x})}{\ln |\vec{x}-\vec{a}|}, \quad L_1(\psi, \vec{a}) := \lim_{|\vec{x}-\vec{a}| \rightarrow 0} [\psi(\vec{x}) - L_0(\psi, \vec{a}) \ln |\vec{x}-\vec{a}|],$$

where  $\alpha_j$  are the (rescaled) coupling constants; the free Hamiltonian corresponds to  $\alpha_j = \infty$ ,  $j = 1, \dots, J$ .

Solvability of the model stems from the fact that one can compute the corresponding resolvent kernel by means of the Krein's formula; all spectral information is contained then in the  $J \times J$  matrix  $\Lambda(z)$  given by

$$\Lambda(z) = \delta_{jm} \left( \alpha_j - \xi(\vec{a}_j; z) \right) - (1 - \delta_{jm}) G_0(\vec{a}_j, \vec{a}_m; z) \quad (3)$$

where  $G_0(\vec{x}_1, \vec{x}_2; z) := \frac{i}{\pi} \sum_{n=1}^{\infty} \frac{e^{ik_n(z)|x_1-x_2|}}{k_n(z)} \sin(ny_1) \sin(ny_2)$  is the free Green's function,  $k_n(z) := \sqrt{z-n^2}$ , and

$$\xi(\vec{a}; z) := \lim_{|\vec{x}-\vec{a}| \rightarrow 0} \left( G_0(\vec{a}, \vec{x}; z) - \frac{1}{2\pi} \ln |\vec{x}-\vec{a}| \right) = \frac{i}{\pi} \sum_{n=1}^{\infty} \left( \frac{\sin^2(nb)}{k_n(z)} - \frac{1}{2in} \right). \quad (4)$$

We suppose everywhere that the energy stays away of the thresholds,  $\sqrt{z} \neq 1, 2, \dots$ . The knowledge of the resolvent allows us, in particular, to solve the scattering problem. The reflection and transmission amplitudes are expressed through the inverse of  $\Lambda(z)$  as

$$r_{nm}(z) = \frac{i}{\pi} \sum_{j,k=1}^J \Lambda(z)_{jk}^{-1} \frac{\sin(mb_j) \sin(nb_k)}{k_m(z)} e^{i(k_m a_j + k_n a_k)}, \quad (5)$$

$$t_{nm}(z) = \delta_{nm} + \frac{i}{\pi} \sum_{j,k=1}^J \Lambda(z)_{jk}^{-1} \frac{\sin(mb_j) \sin(nb_k)}{k_m(z)} e^{-i(k_m a_j - k_n a_k)}.$$

The mirrored quantities are obtained by changing each perturbation longitudinal coordinate  $a_j$  to  $-a_j$ ; together they satisfy the unitarity condition

$$\sum_{m=1}^{[\sqrt{z}]} k_m (t_{nm} \bar{t}_{sm} + r_{nm} \bar{r}_{sm}) = \delta_{ns} k_n, \quad \sum_{m=1}^{[\sqrt{z}]} k_m (\tilde{t}_{nm} \bar{r}_{sm} + \tilde{r}_{nm} \bar{t}_{sm}) = 0,$$

where the summation runs over the open channels,  $[\cdot]$  being the integer part.

### 3 Comparison of the S-matrices

From now on we shall consider a pair of point interactions,  $J = 2$ , with  $a_1 = 0$  and  $a_2 = a$ . For the sake of brevity we denote  $\gamma_j :=$

$\alpha_j - \xi(\vec{a}_j; z)$  and  $G := G_0(\vec{a}_1, \vec{a}_2; z)$ , so the matrix  $\Lambda(z)$  may be written as  $\begin{pmatrix} \gamma_1 & -G \\ -G & \gamma_2 \end{pmatrix}$ . For further purposes we introduce also the truncated resolvent

$$G^t \equiv G_0^t(\vec{a}_1, \vec{a}_2; z) := \frac{i}{\pi} \sum_{n=1}^M \frac{\sin(nb_1) \sin(nb_2)}{k_n(z)} e^{ik_n a}; \quad (6)$$

among the  $M$  modes involved,  $N := \lfloor \sqrt{z} \rfloor$  are propagating while the rest corresponds to evanescent channels. The one-perturbation reflection and transmission are

$$r_{nm}^{(j)} = \frac{i}{\pi} \frac{\sin(nb_j) \sin(mb_j)}{k_m \gamma_j} e^{i(k_n + k_m)a_j}, \quad t_{nm}^{(j)} = \delta_{nm} + \frac{i}{\pi} \frac{\sin(nb_j) \sin(mb_j)}{k_m \gamma_j} e^{i(k_n - k_m)a_j} \quad (7)$$

for  $j = 1, 2$ . Suppose that we employ an  $M$  component Ansatz for wavefunctions in the intermediate region,  $0 < x < a$ . Using the definition (6), we find

$$\left(1 - \tilde{r}^{(1)} r^{(2)}\right)_{nm} = \delta_{nm} - \frac{i}{\pi} G^t \frac{\sin(nb_1) \sin(mb_2)}{k_m \gamma_1 \gamma_2} e^{ik_m a}.$$

This  $M \times M$  matrix is explicitly invertible,

$$\left(1 - \tilde{r}^{(1)} r^{(2)}\right)_{nm}^{-1} = \delta_{nm} + \frac{i}{\pi} \frac{G^t}{\gamma_1 \gamma_2 - (G^t)^2} \frac{\sin(nb_1) \sin(mb_2)}{k_m} e^{ik_m a}. \quad (8)$$

The relations (7) and (8) allow us to express the composed transmission amplitude as the lower left element of the matrix (2); after a straightforward computation using the definition (6), we arrive at the formula

$$t_{nm}^{(12)} = \delta_{nm} + \frac{i}{\pi} \frac{k_m^{-1}}{\gamma_1 \gamma_2 - (G^t)^2} \left\{ \gamma_2 \sin(nb_1) \sin(mb_1) + G^t \sin(nb_2) \sin(mb_1) e^{ik_n a} \right. \\ \left. + G^t \sin(nb_1) \sin(mb_2) e^{-ik_m a} + \gamma_1 \sin(nb_2) \sin(mb_2) e^{i(k_n - k_m)a} \right\}, \quad (9)$$

which differs from the exact expression (5) just by replacing the “*off-diagonal*” coefficients  $G$  by the truncated one  $G^t$ . A similar conclusion

can be made for the other amplitudes in (2). Let us estimate the error due to neglecting the remainder term

$$G^r := \frac{1}{\pi} \sum_{n=M+1}^{\infty} \frac{\sin(nb_1) \sin(nb_2)}{\sqrt{n^2 - z}} e^{-a\sqrt{n^2 - z}}. \quad (10)$$

Denote

$$\tilde{\gamma} := \max\{\gamma_1, \gamma_2\}, \quad \mathcal{D} := \sqrt{(M+1)^2 - (N+1)^2},$$

where the maximum in the first expression is taken over the interval of energies we are interested in. Since  $N = \lfloor \sqrt{z} \rfloor$ , we have

$$(\ell + M + 1)^2 - z \geq (\ell + M + 1)^2 - (N + 1)^2 \geq (\ell + \mathcal{D})^2,$$

and the *relative* error of the “diagonal” terms in (9), *i.e.*, the first and the last one, can be estimated by

$$|\Delta_d| \lesssim \frac{2}{\pi} \left| \frac{G\tilde{\gamma}}{\gamma_1\gamma_2 - (G^t)^2} \right| \sum_{n=M+1}^{\infty} \frac{e^{-a\sqrt{n^2 - z}}}{\sqrt{n^2 - z}} \leq \frac{2}{\pi\mathcal{D}} \left| \frac{G\tilde{\gamma}}{\gamma_1\gamma_2 - (G^t)^2} \right| \frac{e^{-a\mathcal{D}}}{1 - e^{-a\mathcal{D}}};$$

for the off-diagonal ones we have

$$|\Delta_{\text{off}}| \lesssim \frac{1}{\pi\mathcal{D}} \left| \frac{\gamma_1\gamma_2 + G^2}{\gamma_1\gamma_2 - (G^t)^2} \right| \frac{e^{-a\mathcal{D}}}{1 - e^{-a\mathcal{D}}}.$$

This error bounds show where deviations from the exact expression are most likely. An obvious requirement is that the evanescent states must be given opportunity to decay; as long as the moduli are of order of one, it is the exponential term which governs the estimates. To get a  $K$  digit precision, one roughly needs  $(M+1)^2 - (N+1)^2 \gtrsim \left(\frac{K}{2a}\right)^2$ . In general, the problem becomes therefore non-trivial when we glue scatterers without intermediate regions; then one has to check that the evanescent states do indeed decay within each  $S_j$  when we move from its centre to the boundaries.

The second source of error are the denominators. The two-impurity system has no embedded eigenvalues (apart from the trivial ones due to symmetry), so the exact  $\gamma_1\gamma_2 - G^2$  is never zero in the cases of interest



[18]. On the other hand, it has resonances unless the impurity sits at a node of a transverse eigenfunction; they are narrow in the case of a weak coupling, *i.e.*, for  $\alpha_j$  large positive. The truncated expression may blow up around the resonance energies, and even if it is not the case, it may produce shifted resonances. This is important, because resonance structures such as conductivity modulations around thresholds are a primary object of interest in quantum-wire serial scatterers.

To illustrate the differences due to the cut-off factorization, let us compute the conductivity of the quantum wire with a pair of impurities,

$$g(z) = \frac{2e^2}{h} \sum_{n,m=1}^{[\sqrt{z}]} \frac{k_m}{k_n} |t_{nm}(z; M)|^2, \quad (11)$$

where  $t_{nm}(z; M)$  is given by (9) with the resolvent (6) which includes  $M - N$  evanescent states; the limit  $M \rightarrow \infty$  gives the exact answer. Let us remark that the one-point problem contains also a sum over all modes in the function (4) but this can be controlled [18]. We see that even if the approximations with low number of evanescent modes *i.e.*  $M \lesssim 5$  differ considerably only in the vicinity of the thresholds, there are regions like those close to a resonance (*cf.* the inset), where the convergence slows rapidly down. For instance, in order to get the correct position of the peak, higher evanescent modes, up to  $M = 15$  in this particular case, must be taken into account.

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**Figure caption:**

Figure 1: A pair of scatteres.

Figure 2: A pair of point scatteres in the strip.

Figure 3: Conductivity plots for factorized *vs.* exact scattering matrices. The positions of scatterers are  $\vec{a}_1 = (0, \pi/3)$ ,  $\vec{a}_2 = (0.05, 2\pi/3)$  and the coupling constants are chosen  $\alpha_1 = \alpha_2 = 0.2$ . The full line represents the exact result, dotted, dash-dotted and dashed lines the approximations with  $M = 1$ ,  $M = 2$  and  $M = 4$ , respectively. In the inset, however, they represent the approximations with  $M = 5$ ,  $M = 10$  and  $M = 15$ , respectively.

Figure 3

