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METHODOLOGICAL NOTES

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Reduction of the scattering matrix array

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Contents

Abstract. **The scattering matrix approach is widely applied in wave engineering and quantum physics. Usually, a combination of multiple scattering matrices is used. In this article, we consider arbitrary arrays of interconnected scattering matrices and present a formal result for the reduced scattering matrix. We demonstrate this approach in two well-known scattering problems.**

Keywords: scattering matrix, reduction, ballistic regime, double-barrier potential, Aharonov–Bohm effect

1. Introduction

The development of electronic engineering over the last two decades has given rise to the creation of structures containing only a few thousand or even a few hundred atoms. It is sometimes possible to produce coherent structures in which the scattering length of any inelastic collision exceeds the system size. They can be created based on a two-dimensional electron gas in heterostructures [1, 2], specially fabricated nanowires [3], graphene [4], or carbon nanotubes [5]. Such systems are very convenient for manipulating the individual quantum states (for example, using Fabry–Pérot type resonators [6–8]) and producing devices based on the nonlocality of quantum mechanics [9, 10].

Coherent systems can be conveniently described by scattering matrices [11]. In addition, such an approach is widely used in wave mechanics, in particular, for designing microwave devices [12]. In this field, the scattering matrix approach is already a well-developed engineering tool. In quantum electronics, however, such a systematization is actually lacking. In this paper, we present a systematic scattering matrix approach for the determination of the arrays of arbitrarily connected scatterers.

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2. Scattering matrix array

Let us consider a set of scattering matrices $\{\mathcal{S}_1, \mathcal{S}_2, \ldots\}$ coupling input $|\mathrm{I}_\alpha\rangle$ and output $|\mathrm{O}_\alpha\rangle$ states: $|\mathrm{O}_\alpha\rangle = \mathcal{S}_\alpha |\mathrm{I}_\alpha\rangle$. Each of the matrices $\mathcal{S}_\alpha$ ($\alpha = 1, 2, \ldots$) is unitary, $\mathcal{S}_\alpha^\dagger \mathcal{S}_\alpha = 1$, and has the size $n_\alpha \times n_\alpha$. Let us introduce a notion of the scattering matrix of a whole system, or a *grand* scattering matrix $\mathcal{S}$ of size $n \times n$, where $n = \sum_\alpha n_\alpha$, which couples all the input $|\mathrm{I}\rangle$ and output $|\mathrm{O}\rangle$ states, namely

$$|\mathrm{I}\rangle = \mathcal{S}|\mathrm{O}\rangle\,, \tag{1}$$

where

$$\mathcal{S} \equiv \begin{bmatrix} \mathcal{S}_1 & & & \\ & \mathcal{S}_2 & & \\ & & \mathcal{S}_3 & \\ & & & \ddots \end{bmatrix}, \quad |\mathrm{I}\rangle \equiv \begin{bmatrix} |\mathrm{I}_1\rangle \\ |\mathrm{I}_2\rangle \\ |\mathrm{I}_3\rangle \\ \vdots \end{bmatrix}, \quad |\mathrm{O}\rangle \equiv \begin{bmatrix} |\mathrm{O}_1\rangle \\ |\mathrm{O}_2\rangle \\ |\mathrm{O}_3\rangle \\ \vdots \end{bmatrix} \tag{2}$$

(see the schematic diagram of scattering channels in Fig. 1a). Like scattering matrices $\mathcal{S}_\alpha$, the large scattering matrix $\mathcal{S}$ is unitary, but not necessarily symmetric.

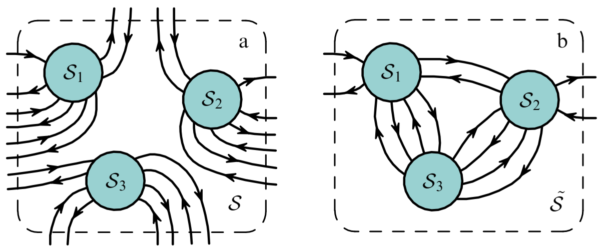

Figure 1. (a) Grand scattering matrix $\mathcal{S}$. (b) Reduced scattering matrix $\tilde{\mathcal{S}}$.

Let all the scatterers be arbitrarily connected into an array as shown in Fig. 1b. Each connection (internal channel) in the scattering matrix array will be described by two indices corresponding to some input and output of the large scattering matrix $\mathcal{S}$. Such a connection reduces the effective size of the grand scattering matrix $\mathcal{S}$ by unity in both dimensions. The case of p connections can be described by specifying the two lists of indices $\{o\}$ and $\{i\}$ of length p such that the output o_1 of the large scattering matrix $\mathcal{S}$ is coupled with its input i_1, the output o_2 with the input i_2, etc. We denote the vectors of input and output states corresponding to indices $\{o\}$ and $\{i\}$ by $|\mathrm{LI}\rangle$ and $|\mathrm{LO}\rangle$, and unite the rest of the elements from $|\mathrm{L}\rangle$ and $|\mathrm{O}\rangle$ in 'external' states $|\mathrm{EI}\rangle$ and $|\mathrm{EO}\rangle$. The $\tilde{\mathcal{S}}$ matrix reduced in this way couples the external states only:

$$|\mathrm{EI}\rangle = \tilde{\mathcal{S}}|\mathrm{EO}\rangle\,. \tag{3}$$

We will call the $\tilde{\mathcal{S}}$ matrix the *reduced* scattering matrix.

3. Reduction of the grand scattering matrix

3.1 Successive reduction

Let us describe the reduction of the grand scattering matrix $\mathcal{S} = \{S_{kl}\}$ with elements S_{kl} in the case of a single connection between the ith input and oth output. We denote the input amplitudes of the large scattering matrix by I_l, and the output amplitudes by O_k so that

$$O_k = \sum_l S_{kl} I_l\,. \tag{4}$$

Let us consider separately coupled contacts:

$$O_o = \sum_{l,\,l\neq i} S_{kl} I_l + S_{oi} I_i\,.$$

The coupling means the equality of the corresponding input and output amplitudes: $I_i = O_o$. Taking this into account, we obtain the equation for the amplitude in the connection site:

$$I_i = O_o = \frac{1}{1 - S_{oi}} \sum_{l,\,l\neq i} S_{kl} I_l\,. \tag{5}$$

By substituting expression (5) into equation (4), we find for $k \neq o$:

$$O_k = \sum_{l,\,l\neq i} \tilde{S}_{kl} I_l\,, \tag{6}$$

where elements of the reduced scattering matrix $\tilde{\mathcal{S}}$ are defined by the expression

$$\tilde{S}_{kl} = S_{kl} + \frac{S_{ki} S_{ol}}{1 - S_{oi}}\,. \tag{7}$$

In this equation, we 'omit' the ith column and oth row of the initial matrix $\mathcal{S}$, so that the dimensions of the reduced matrix $\tilde{\mathcal{S}}$ are $(n-1)\times(n-1)$. By repeating this procedure p times, the initial grand scattering matrix can be reduced to the size $(n-p)\times(n-p)$.

This method can be efficiently applied to a small number of connections. In the case of a large number of connections, we can generalize this method and derive the expression for the reduced scattering matrix in the matrix form corresponding to the successive implementation of the procedure described above.

3.2 Matrix reduction

For the case of p connected channels, let us represent the grand scattering matrix $\mathcal{S}$ in the block form, denoting it by $\hat{\mathcal{S}}$. To this end, we permute elements in grand vectors of the input and output states and correspondingly permute columns and rows in the grand scattering matrix (it is known that unitarity is preserved in this case). Placing all the connected elements in the grand vector of input and output states be at the end of the vector, their order corresponding to the connection order, we obtain

$$\hat{\mathcal{S}} \equiv \begin{bmatrix} \mathcal{S}_{\mathrm{E,E}} & \mathcal{S}_{\mathrm{E,L}} \\ \mathcal{S}_{\mathrm{L,E}} & \mathcal{S}_{\mathrm{L,L}} \end{bmatrix}, \quad \begin{bmatrix} |\mathrm{EO}\rangle \\ |\mathrm{LO}\rangle \end{bmatrix} = \mathcal{S} \begin{bmatrix} |\mathrm{EI}\rangle \\ |\mathrm{LI}\rangle \end{bmatrix}. \tag{8}$$

In fact, the $\hat{\mathcal{S}}$ matrix couples the external output states $|\mathrm{EO}\rangle$ of the reduced system with its external input states $|\mathrm{EI}\rangle$. Equation (8) also comprises the amplitudes at connections $|\mathrm{LO}\rangle$ and $|\mathrm{LI}\rangle$, equal to each other: $|\mathrm{LO}\rangle = |\mathrm{LI}\rangle$. Taking this into account, we can obtain the reduced $(n-p)\times(n-p)$ scattering matrix $\tilde{\mathcal{S}}$ coupling the external output states with the external input states, $|\mathrm{EO}\rangle = \tilde{\mathcal{S}}|\mathrm{EI}\rangle$, so that

$$\tilde{\mathcal{S}} = \mathcal{S}_{\mathrm{E,E}} + \mathcal{S}_{\mathrm{E,L}}(1 - \mathcal{S}_{\mathrm{L,L}})^{-1}\mathcal{S}_{\mathrm{L,E}}\,, \tag{9}$$

where 1 denotes the $n \times n$ unit matrix. This result coincides with expression (7) in the case of one channel. The reduced matrix $\tilde{\mathcal{S}}$ defined by the relationship (9) is unitary, $\tilde{\mathcal{S}}^{\dagger}\tilde{\mathcal{S}} = 1$, the block $\mathcal{S}_{\mathrm{L,L}}$ is square by the construction, and the term $(1 - \mathcal{S}_{\mathrm{L,L}})^{-1}$ is responsible for the poles of the reduced scattering matrix.

3.3 Quantization condition

Let us consider a special case in which the number of connections coincides with the size of the grand scattering matrix: $p = n$. Physically, this corresponds to the absence of inputs and outputs, which means that the wave function will be zero at infinity. As is known from quantum mechanics, the energy levels in such a system will be quantized. Expression (9) obtained in Section 3.2 gives the quantization condition

$$\det(1 - \mathcal{S}_{\mathrm{L,L}}) = 0\,, \tag{10}$$

where $\mathcal{S}_{\mathrm{L,L}}$ coincides with the initial grand scattering matrix $\mathcal{S}$ up to the permutation of rows and columns.

4. Examples

Let us apply the method described in Section 3 to two well-known problems.

4.1 Double-barrier potential

As a first example, let us consider a double-barrier potential formed by two identical point scatterers with the transmission amplitude t and reflect-ion amplitude r separated by the distance L. The scattering matrix of each barrier is given by the expression

$$\mathcal{S}_1 = \mathcal{S}_2 = \begin{bmatrix} r & t \\ t & r \end{bmatrix}.$$

In order to apply the formal approach described above, we introduce the 1×1 scattering matrices corresponding to the motion of a particle with energy E between barriers from left to right and from right to left. These scattering matrices stand for acquiring the same phase:

$$\mathcal{S}_3 = \mathcal{S}_4 = \exp(\mathrm{i}kL),$$

where $k = \sqrt{2mE}/\hbar$. (Matrices $\mathcal{S}_1$ and $\mathcal{S}_2$ are usually presented as a single diagonal scattering matrix, $\mathrm{diag}\{\mathcal{S}_1, \mathcal{S}_2\}$, but we divided it into two for clarity.) The large scattering matrix of the double-barrier potential is given by

$$\mathcal{S} = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{array} \begin{array}{cc|cc|c|c} 1 & 2 & 3 & 4 & 5 & 6 \\ r & t & & & & \\ t & r & & & & \\ \hline & & r & t & & \\ & & t & r & & \\ \hline & & & & \exp(\mathrm{i}kL) & \\ \hline & & & & & \exp(\mathrm{i}kL) \end{array}.$$

We permute the rows and columns of the matrix $\mathcal{S}$ according to formula (8), so that elements in the lower right block correspond to internal connections. The trajectories and numeration of inputs and outputs are presented in Fig. 2. The matrix $\hat{\mathcal{S}}$ will take the form

$$\hat{\mathcal{S}} = \begin{array}{c} \\ 1 \\ 4 \\ 5 \\ 3 \\ 2 \\ 6 \end{array} \begin{array}{cc|cccc} 1 & 4 & 2 & 5 & 6 & 3 \\ r & & t & & & \\ & r & & & & t \\ \hline & & & \exp(\mathrm{i}kL) & & \\ & t & & & & r \\ t & & r & & & \\ & & & & \exp(\mathrm{i}kL) & \end{array}.$$

Then, following the method described, we calculate the inverse matrix

$$(1 - \mathcal{S}_{\mathrm{L,L}})^{-1} = \frac{1}{1 - r^2 \exp(2\mathrm{i}kL)}$$

$$\times \begin{bmatrix} 1 & \exp(\mathrm{i}kL) & r\exp(2\mathrm{i}kL) & r\exp(\mathrm{i}kL) \\ r^2\exp(\mathrm{i}kL) & 1 & r\exp(\mathrm{i}kL) & r \\ r & r\exp(\mathrm{i}kL) & 1 & r^2\exp(\mathrm{i}kL) \\ r\exp(\mathrm{i}kL) & r\exp(2\mathrm{i}kL) & \exp(\mathrm{i}kL) & 1 \end{bmatrix},$$

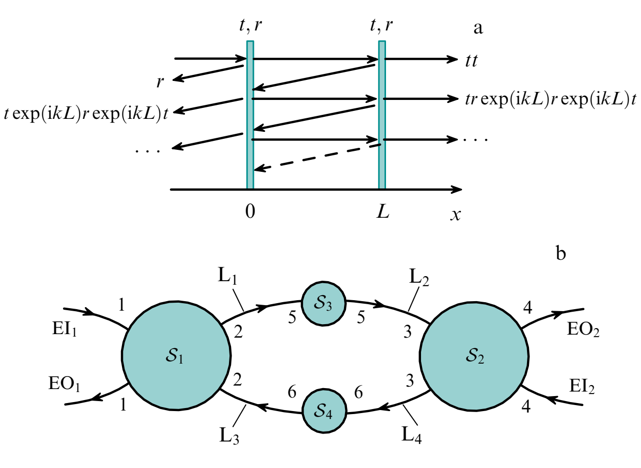

Figure 2. Fabry–Pérot interferometer: (a) structure and trajectories in a double-barrier potential, and (b) equivalent scattering matrix array.

and, by substituting it into expression (9), obtain the known result for the double-barrier potential [11, 13]:

$$\tilde{\mathcal{S}} = \begin{bmatrix} \dfrac{t^2\exp(\mathrm{i}kL)}{1 - r^2\exp(2\mathrm{i}kL)} & r + \dfrac{rt^2\exp(\mathrm{i}kL)}{1 - r^2\exp(2\mathrm{i}kL)} \\[3ex] r + \dfrac{rt^2\exp(\mathrm{i}kL)}{1 - r^2\exp(2\mathrm{i}kL)} & \dfrac{t^2\exp(\mathrm{i}kL)}{1 - r^2\exp(2\mathrm{i}kL)} \end{bmatrix}.$$

Note that this result for the double-barrier potential can be rather simply generalized to the case of a multibarrier potential by recursive substitution. In order to calculate transport properties of the scatterers connected in series, one may use transfer matrices coupling the states on the left and on the right of each scatterer. The resulting transfer matrix of the system is then a multiplication of all individual transfer matrices. However, this approach is invalid for a more complicated topology of connected scatterers.

4.2 Aharonov–Bohm effect

To demonstrate the reduction of the scattering matrix array in a more complex topology, we will employ it to describe the well-known Aharonov–Bohm effect [14]. Let us consider a system consisting of a coherent conductor closed in a loop as shown in Fig. 3a. The ring is threaded by a magnetic flux Φ. For simplicity, we consider the classic situation without backward reflection and in the absence of energy-dependent resonances. This can be realized with the help of specular reflection, as illustrated in Fig. 3b.

Naively, one can expect scattering matrices $\mathcal{S}_1$ and $\mathcal{S}_2$ describing splitters to be of size 3×3. However, 3×3 scattering matrices cannot describe back reflectionless case. It is easy to check by parametrizing such a scattering matrix with a minimum set of independent parameters [15, 16]. In order to correctly describe a back reflectionless scatterer, it is required to consider at least the 4×4 scattering matrix (Fig. 3c). The required form of the matrix can be easily obtained by demanding: (1) the absence of backward scattering in all channels; (2) the absence of scattering from the upper wire to the lower one and vice versa, and (3) the left-to-right symmetry. These conditions give expressions for the

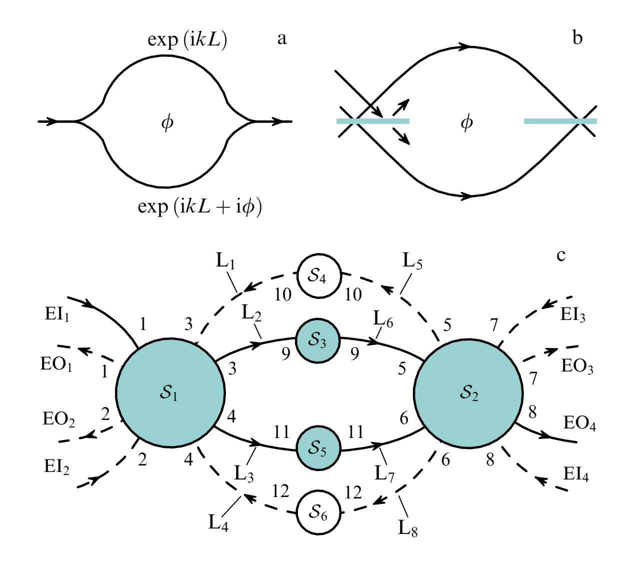

Figure 3. Aharonov–Bohm effect: (a) classical scheme, (b) realization of reflectionless scatterers, and (c) equivalent scattering matrix array.

scattering matrices of the left and right ‘Y-splitters’:

$$\mathcal{S}_1 = \mathcal{S}_2 = \left[\begin{array}{cc|cc} & & r & t \\ & & t & r \\ \hline r & t & & \\ t & r & & \end{array}\right].$$

The magnetic flux Φ is modelled by the additional phase $\phi = 2\pi\Phi/\Phi_0$ (where Φ_0 is a magnetic flux quantum) in the scattering matrix of the upper arm, $\mathcal{S}_3 = \mathcal{S}_4 = f \equiv \exp(\mathrm{i}\phi + \mathrm{i}kL)$, with respect to the lower one, $\mathcal{S}_5 = \mathcal{S}_6 = g \equiv \exp(\mathrm{i}kL)$. By collecting all these matrices to the grand scattering matrix $\mathcal{S} = \mathrm{diag}\{\mathcal{S}_1, \ldots, \mathcal{S}_6\}$ and permuting its rows and columns in accordance with formula (8), we obtain

$$\hat{\mathcal{S}} = \begin{array}{c} \\ 1 \\ 2 \\ 7 \\ 8 \\ 3 \\ 9 \\ 11 \\ 4 \\ 10 \\ 5 \\ 6 \\ 12 \end{array} \begin{array}{cccc|cccccccc} 1 & 2 & 7 & 8 & 10 & 3 & 4 & 12 & 5 & 9 & 11 & 6 \\ & & & & & r & t & & & & & \\ & & & & & t & r & & & & & \\ & & & & & & & & r & & & t \\ & & & & & & & & t & & & r \\ \hline r & t & & & & & & & & & & \\ & & & & & & & & & f & & \\ & & & & & & & & & & g & \\ t & r & & & & & & & & & & \\ & & & & f & & & & & & & \\ & & r & t & & & & & & & & \\ & & t & r & & & & & & & & \\ & & & & & & & g & & & & \end{array}.$$

Then, by substituting the blocks of the matrix $\hat{\mathcal{S}}$ into formula (9), we find the reduced scattering matrix

$$\tilde{\mathcal{S}} = \begin{bmatrix} & & fr^2 + gt^2 & (f+g)\,rt \\ & & (f+g)\,rt & gr^2 + ft^2 \\ fr^2 + gt^2 & (f+g)\,rt & & \\ (f+g)\,rt & gr^2 + ft^2 & & \end{bmatrix}.$$

The transmission amplitude is given by the expression $a = gr^2 + ft^2 = \exp(\mathrm{i}kL)[r^2 + t^2 \exp(\mathrm{i}\phi)]$. For the symmetric case, $t = 1/\sqrt{2}$ and $r = -\mathrm{i}/\sqrt{2}$, the corresponding transmission probability $A = |a|^2 = (1 - \cos\phi)/2$ gives the known result for the Aharonov–Bohm effect.

5. Conclusions

In wave physics, and in accelerator physics in particular, there is a method similar to the described above, which is called the mode matching technique [17]. This technique was utilized in different specialized software, which allows simulating parts of the waveguide. For example, the typical system is a series connection of two waveguides with a large number of channels. In this case, the continuity of the longitudinal and transverse components of fields gives a system of linear equations resembling the definition (1), (2) of the large scattering matrix. The more general procedure of ‘joining’ two scattering matrices for the description of microwave devices (in other words, the addition of one element to the waveguide construction) is presented in thesis [18]. This procedure resembles the step-by-step reduction described in Section 3.

It should be noted that the reduction procedure of the scattering matrix can be applied to hybrid systems with superconducting parts [19] by considering the total or partial Andreev reflection. Electric circuits with Andreev reflection are considered in detail in paper [20].

In principle, the scattering matrix reduction method does not require the unitarity of initial scattering matrices. For, example, in Section 4.2 one would describe a ‘Y-splitter’ and a ‘Y-mixer’ by 1×2 and 2×1 matrices, respectively. Such an approach gives the same result for the scattering amplitudes, but, strictly speaking, neglects the flow conservation and therefore does not require the unitarity of matrices. This approach can considerably reduce the calculation time; however, it does not offer a procedure for verifying calculations by testing the unitarity of the reduced scattering matrix.

Summing up, we have demonstrated the systematic approach to calculating scattering matrices for mesoscopic systems. We have presented the analytical result for the reduced scattering matrix and have tested it on known physical systems. The main advantage of the method described is its convenience for numerical implementation.

6. Appendix. Numerical realization

The reduction procedure described by expressions (8) and (9) utilizes successive indexing of inputs and outputs. In practice, it is more convenient to employ compounded indexing involving the scattering matrix number and the input (output) number in the matrix. Such indexing is used in MATLAB Listing 1. The function presented accepts scattering matrix array `Ss`, the coupling array `Ls`, and the input state array `Is` as arguments, and returns output state array `Os`.

Let us test this function on the double-barrier potential. The corresponding code is presented in Listing 2. It calculates

```
function [Os,Is] = reduceScatteringMatrix(Ss,Ls,Is)
  Ns = zeros(length(Ss),1); Ms = zeros(length(Ss),1);
  nz = 0;
  for s=1:length(Ss)-1,
    Ns(s+1) = Ns(s) + size(Ss{s},1);
    Ms(s+1) = Ms(s) + size(Ss{s},2);
    nz = nz + numel(Ss{s});
  end
  N = Ns(end) + size(Ss{end},1);
  M = Ms(end) + size(Ss{end},2);

  S = sparse([],[],[],N,M,nz);
  I = zeros(M,1);  O = zeros(N,1);
  for s = 1:length(Ss),
    S(Ns(s)+1:Ns(s)+size(Ss{s},1), ...
      Ms(s)+1:Ms(s)+size(Ss{s},2)) = Ss{s};
    I(Ms(s)+1:Ms(s)+size(Ss{s},2)) = Is{s};
  end

  LOi = NaN(length(Ls),1); LIi = NaN(length(Ls),1);
  for l = 1:length(Ls),
    L = Ls{l};
    n = L(1); i = L(2); m = L(3); j = L(4);
    po = Ns(n)+i; pi = Ms(m)+j;
    O(po) = NaN; I(pi) = NaN;
    LOi(l) = po; LIi(l) = pi;
  end

  u = (speye(length(Ls)) - S(LOi,LIi)) \ ...
    (S(LOi,~isnan(I))*I(~isnan(I)));

  O(~isnan(O)) = S(~isnan(O),LIi)*u + ...
    S(~isnan(O),~isnan(I))*I(~isnan(I));

  O(LOi) = u;  I(LIi) = u;

  Os = cell(1,length(Ss));
  for s = 1:length(Ss),
    Is{s} = I(Ms(s)+1:Ms(s)+size(Ss{s},2));
    Os{s} = O(Ns(s)+1:Ns(s)+size(Ss{s},1));
  end
end
```

Listing 1. MATLAB realization of the scattering matrix reduction.

```
kLs = 0:0.01:2*pi; Ts = NaN(size(kLs));
for e = 1:length(kLs),
  kL = kLs(e);
  Ss = cell(1,4); Ls = cell(1,4); Is = {};

  t = sqrt(0.1); r = 1i*sqrt(1-abs(t)^2);
  Ss{1} = [r t; t r];  Is{1} = [1; NaN];
  Ss{2} = [r t; t r];  Is{2} = [0; NaN];
  Ss{3} = exp(1i*kL);  Is{3} = NaN;
  Ss{4} = exp(1i*kL);  Is{4} = NaN;

  Ls{1} = [1 2  4 1];
  Ls{2} = [4 1  2 2];
  Ls{3} = [2 2  3 1];
  Ls{4} = [3 1  1 2];

  Os = reduceScatteringMatrix(Ss, Ls, Is);
  Ts(e) = abs(Os{2}(1))^2;
end
plot(kLs/(2*pi), Ts);
```

Listing 2. Calculation of the transparency of a double-barrier potential using the scattering matrix reduction.

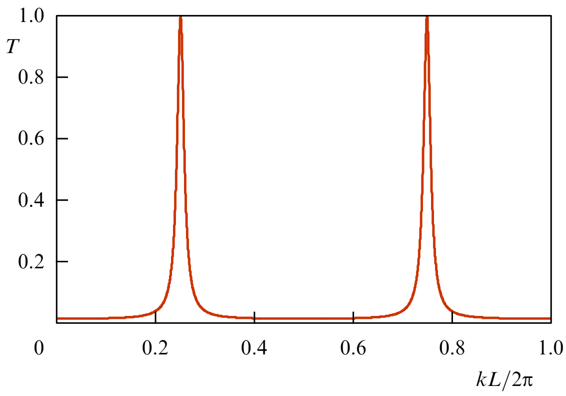

Figure 4. Transparency of a double-barrier potential as a function of phase kL.

the dependence of the transparency of the double-barrier potential on the phase kL, and plots the result as shown in Fig. 4.

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