Useful equation of tridiagonal matrices in application to electron transport through a quantum wire

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Abstract

In this paper the transmittance through a quantum wire connected with two electron reservoirs is calculated and non-trivial transformation between the evolution operator method and the Green’s function technique is reported. To show this equivalence an analytical non-linear formula which concerns symmetrical tridiagonal matrices is proofed. This formula connects the cofactor and three determinants of tridiagonal matrices.

1 Introduction

There are many mathematical, e.g. [1, 2, 3], and physical, e.g. [3, 4, 5, 6], problems which are described by means of tridiagonal matrices. For such matrices many analytical properties were reported especially to find the determinant or the inverse of this kind of matrices, cf. Refs. [3, 7, 8, 9, 10]. These properties allows us to derive analytically many physical and mathematical problems. In
this work we report one interesting equation which concerns symmetric tridiagonal matrices. This equation can be useful in obtaining solutions of many mathematical and physical problems with tridiagonal matrices and finally it can lead to analytical expressions for physical quantities or in mathematical calculations.

As an example of this equation we obtain the transmittance through a quantum wire between two eternal electrodes. Electronic properties of quantum wires are very important mainly from the practical point of view i.e. due to their potential applications in nanoelectronic - they are the thinnest possible electric conductors. We obtain the transmittance through a wire by means of the evolution operator (EO) method and show that the final analytical relation for the transmittance is the same as that one obtained within the Green’s function (GF) technique. Note, that there is no trivial transformation between the final results obtained within these methods. Until now, analytical derivation of the quantum wire transmittance, obtained by means of the evolution operator method, was not reported in the literature.

2 Nonlinear relation on tridiagonal matrixes

Lets consider tridiagonal symmetrical square matrix $A_N$ (dimension $N \times N$) written in the following form:

$$A_N = \begin{pmatrix}
\alpha & \beta & 0 & 0 & \cdots & 0 \\
\beta & \alpha & \beta & 0 \\
0 & \beta & \alpha & \beta \\
0 & 0 & \beta & \alpha \\
\vdots & \ddots & \ddots & \ddots \\
0 & & & & & \alpha
\end{pmatrix}_{N \times N}$$

(1)

where $\alpha$ and $\beta$ are real numbers. For this matrix the following nonlinear equation is satisfied:

$$[\text{cof}(A_N)_{N,1}]^2 = A_{N-1}^2 - A_{N-2}A_N$$

(2)

where $A_N$ is the determinant of $A_N$ matrix, $A_N = \det A_N$, (we consider $A_N \neq 0$) and $\text{cof}(A_N)_{N,1}$ means the algebraic complement (cofactor) of $A_N$ matrix versus the element $(N,1)$ or $(1,N)$. Note, that Eq. 2 connects the cofactor of the matrix $A_N$ and three determinants of this matrix for different
dimensions, i.e. $N, N-1$ and $N-2$. It is interesting that this relation is connected with the Fibonacci and Lucas numbers, e.g. [15] [16], where only the integer numbers appear and, moreover, it can be transformed to a kind of trigonometrical relation because the determinant of tridiagonal matrixes can be expressed by means of the second kind Chebyshev polynomials. Here we show a simple proof of this relation using only well known properties of tridiagonal matrixes with arbitrary real $\alpha$ and $\beta$.

**Proof of Eq. 2.** The cofactor in Eq. 2 can be expressed as follows:

$$\text{cof}(A_N)_{N,1} \equiv B_{N-1} = \det \begin{pmatrix} \beta & 0 & 0 & \cdots & 0 \\ \alpha & \beta & 0 & \cdots & 0 \\ \beta & \alpha & \beta & 0 & \cdots \\ 0 & \beta & \alpha & \beta & 0 \\ \vdots & & & \ddots & \beta \end{pmatrix}_{N-1 \times N-1}$$

Using Eq. 3 the left side of Eq. 2 can be expressed only by means of $\beta$ elements and the dimension of the matrix $A_N$, i.e.

$$[\text{cof}(A_N)_{N,1}]^2 = B_{N-1}^2 = \beta^{2N-2}$$

Now, we proof that the right side of Eq. 2 can be also expressed in the same form. In our calculation we use the following recurrence relation, e.g. [4] [8],

$$A_N = \alpha A_{N-1} - \beta^2 A_{N-2}$$

Using this equation the right side of Eq. 2 can be written as follows:

$$A_{N-1}^2 - A_{N-2} A_N = (\alpha A_{N-2} - \beta^2 A_{N-3})^2 - A_{N-2}(\alpha^2 A_{N-2} - \alpha \beta^2 A_{N-3} - \beta^2 A_{N-2})$$

and after some algebra one obtains

$$\beta^2(A_{N-2}^2 - A_{N-3} A_{N-1})$$

which is also the recurrence relation and in the end it leads to the final result for the right side of Eq. 2

$$\beta^{2(N-2)}(A_1^2 - A_0 A_2) = \beta^{2N-2}$$

Here we use the explicate forms of $A_N$ determinants, i.e. $A_2 = \alpha^2 - \beta^2$, $A_1 = \alpha$ and $A_0 = 1$. The last result, Eq. 8, is the same one as Eq. 4 (obtained for the left side of Eq. 2). Thus the main equation of this paper, Eq. 2, has been proofed.■
3 Electron transport through a quantum wire

In this section we consider the electron transport through a quantum wire coupled with the left and right electrodes. The wire is represented by a finite, straight chain of \( N \) sites with the nearest-neighbour hoppings, i.e. electrons cannot tunnel between the next-neighbour sites. For simplicity we consider the case of no electron-electron correlations. The Hamiltonian of considered system, written in the second quantization notation, is given by

\[
H = H_0 + V,
\]

where

\[
H_0 = \sum_{\vec{k} \alpha = L,R} \varepsilon_{\vec{k} \alpha} c_{\vec{k} \alpha}^+ c_{\vec{k} \alpha} + \sum_{i=1}^{N} \varepsilon_0 c_i^+ c_i,
\]

is a single electron Hamiltonian which stands for on-site energies and

\[
V = \sum_{\vec{k} L} V_{\vec{k} L} c_{\vec{k} L}^+ c_1 + \sum_{\vec{k} R} V_{\vec{k} R} c_{\vec{k} R}^+ c_N + \sum_{i=1}^{N-1} V_N c_i^+ c_{i+1} + \text{h.c.}
\]

represents the interaction energy. Here the operators \( c_{\vec{k} \alpha} (c_{\vec{k} \alpha}^+) \), \( c_i (c_i^+) \) are the annihilation (creation) operators of the electron in the lead \( \alpha (\alpha = L, R) \) and at site \( i \) in the wire, respectively. The wire sites are described by the electron energy levels, \( \varepsilon_0 \), which are the same for all sites. Our wire is coupled to both electrodes through the tunneling barriers with the transfer-matrix elements \( V_{\vec{k} L} \) (the first wire site: \( i = 1 \)) and \( V_{\vec{k} R} \) (the last wire site: \( i = N \)). \( V_N \) denotes the hopping integrals between the nearest-neighbour wire sites and are the same for all sites. In the above Hamiltonian \( \varepsilon_{\vec{k} L/R} \) corresponds to the energy of electrons with the wave vector \( \vec{k} \) in the left or right electrodes.

3.1 Green’s function method

For considered here system the transmittance, \( T(\varepsilon) \), can be expressed by means of the retarded Green’s function between the first and the last quantum wire sites, \( G_{1N}^r(\varepsilon) \), cf. [4, 5, 6]:

\[
T(\varepsilon) = \Gamma^2 |G_{1N}^r(\varepsilon)|^2
\]

Using equation of motion for the retarded Green’s function and the Hamiltonian of the system one can find the following relation for the element \( G_{1N}^r(\varepsilon) \):

\[
G_{1N}^r(\varepsilon) = \frac{\text{cof}(C_N)_{N,1}}{C_N}
\]
where $C_N$ is a kind of symmetric tridiagonal matrix ($C_N$ is its determinant) and can be written in the form

$$
C_N = \begin{pmatrix}
\varepsilon_0 - \varepsilon_{\vec{k}L} & -V_N & 0 & \cdots & 0 \\
-V_N & \varepsilon_0 - \varepsilon_{\vec{k}L} & -V_N & & \\
0 & -V_N & \varepsilon_0 - \varepsilon_{\vec{k}L} & \ddots & \\
& \ddots & \ddots & \ddots & \\
0 & & & & \varepsilon_0 - \varepsilon_{\vec{k}L} + i\frac{\Gamma}{2}
\end{pmatrix}_{N \times N}
$$

(13)

Here we use the wide-band limit approximation i.e. \( \Gamma = \frac{\Gamma}{L/R} = 2\pi \sum_{\vec{k}L} V_{\vec{k}L} V_{\vec{k}L}^* \delta(\varepsilon - \varepsilon_{\vec{k}L}) = 2\pi |V_L|^2 / D \) where we assume that $V_{\vec{k}L}$ elements do not depend on the wave vector $\vec{k}\alpha$ ($V_{\vec{k}\alpha} = V_{\alpha}$) and $D$ is the effective band width of the left electrode. Using Eq. (12) the transmittance can be written as follows:

$$
T(E) = \Gamma^2 \frac{|\text{cof}(C_N)_{N,1}|^2}{|C_N|^2}
$$

(14)

It is worth noting that the determinant of the matrix $C_N$ as well as the cofactor can be obtained analytically which leads to the analytical formula for the transmittance, see e.g. [4].

### 3.2 Evolution operator technique

In this subsection we obtain the transmittance through the wire using the evolution operator method. The current flowing through the system (or the transmittance) can be expressed by means of appropriate evolution operator matrix elements, e.g. [11, 12], i.e.

$$
j_L(t) = -e \frac{dn_L(t)}{dt} = -e \frac{d}{dt} \sum_{\vec{k}L} n_{\vec{k}L}(t) = \sum_{\vec{k}L} \sum_\beta n_\beta(t_0) |U_{\vec{k}L,\beta}(t, t_0)|^2
$$

(15)

where $n_L(t)$ means the electron occupation of the left electrode at time $t$, $n_\beta(t_0)$ represents the initial filling of the corresponding single-particle states ($\beta = i, \vec{k}L, \vec{k}R$) and $U(t, t_0)$ is the evolution operator matrix element which satisfies the following equation of motion (in the interaction representation, $\hbar = 1$), cf. [11, 13, 14]:

$$
i \frac{\partial}{\partial t} U(t, t_0) = \tilde{V}(t) U(t, t_0)
$$

(16)
Here $\tilde{V}(t) = U_0(t, t_0) V(t) U_0^*(t, t_0)$ and $U_0(t, t_0) = T \exp \left( i \int_{t_0}^{t} dt' H_0(t') \right)$. Assuming the wide band limit approximation the current, Eq. 15, can be written in the following form:

$$j_L(t) = -\Gamma_L \left( \sum_{kL} n_{kL}(0) |U_{1\tilde{k}L}(t)|^2 + \sum_{kR} n_{kR}(0) |U_{1\tilde{k}R}(t)|^2 \right) - 2 \text{Im} \left( V_L \sum_{kL} n_{kL}(0) e^{i(\epsilon_{kL} - \epsilon_1) t} U_{1\tilde{k}L}(t) \right) \tag{17}$$

To obtain the transmittance, one can symmetrize the average current flowing through the system:

$$\langle j(t) \rangle = \langle j_L(t) \rangle = (\langle j_L(t) \rangle - \langle j_R(t) \rangle) / 2$$

and finally we find the Landauer formula for the current:

$$\langle j(t) \rangle = \int d\epsilon (f_L(\epsilon) - f_R(\epsilon)) T(\epsilon) \tag{18}$$

where the transmittance, $T(\epsilon)$, is expressed by means of the evolution operator elements:

$$T(\epsilon) = \frac{\Gamma_L}{2D} \left( |\langle U_{N,kL}(t) \rangle|^2 - |\langle U_{1\tilde{k}L}(t) \rangle|^2 \right) - \text{Im} \frac{V_L}{D} \langle e^{i(\epsilon_0 - \epsilon_{kL}) t} U_{1\tilde{k}L}(t) \rangle \tag{19}$$

These elements satisfy the following set of differential equations

$$\frac{\partial}{\partial t} U_{i,\tilde{k}L}(t) = -iV_N (U_{i+1,\tilde{k}L}(t) + U_{i-1,\tilde{k}L}(t)) - \delta_{i,1} \left( iV_L e^{i(\epsilon_0 - \epsilon_{kL}) t} + \Gamma_L U_{1\tilde{k}L}(t)/2 \right) - \delta_{i,N} \Gamma_R U_{N,\tilde{k}L}(t)/2 \tag{20}$$

Note, that there are $N$ complex equations and for $N = 1$ or $N = 2$ simple analytical solutions for $U_{i,\tilde{k}L}(t)$ exist. In general, for arbitrary $N$, it can be shown that the above set of differential equations can be written in the following matrix notation:

$$\mathbf{C}_N \dot{\mathbf{U}} = \dot{\mathbf{J}} \tag{21}$$

where $\mathbf{C}_N$ is defined according to Eq. 13, $\dot{\mathbf{U}}$ is $N$-element vector, $\mathbf{U} = [U_{1,\tilde{k}L}(t), \ldots, U_{N,\tilde{k}L}(t)]_N$ and $\dot{\mathbf{J}} = [iV_L e^{i(\epsilon_0 - \epsilon_{kL}) t}, 0, \ldots, 0]_N$. The formal solution for the evolution operator matrix elements reads:

$$U_{i,\tilde{k}L}(t) = (\mathbf{C}_N)^{-1} iV_L e^{i(\epsilon_0 - \epsilon_{kL}) t} \tag{22}$$
where $(C_N)_{i,1}^{-1}$ means $(i,1)$ element of the inverse matrix $(C_N)^{-1}$. Using the above solution we find that:

$$\langle |U_{1,\vec{k}L}(t)|^2 \rangle = 2\pi V_L^2 \frac{|\hat{C}_{N-1} + i\frac{\Gamma}{2}\hat{C}_{N-2}|^2}{|C_N|^2}$$ \hfill (23)

$$\langle |U_{N,\vec{k}L}(t)|^2 \rangle = 2\pi V_L^2 \frac{|\text{cof}(C_N)_{N,1}|^2}{|C_N|^2}$$ \hfill (24)

$$- \text{Im} \frac{V_L}{D} \langle e^{i(\epsilon - \epsilon_0)t}U_{1,\vec{k}L}(t) \rangle = \frac{\Gamma^2}{2|C_N|^2} \left(2\hat{C}_{N-1}^2 - \hat{C}_{N-2}\hat{C}_N + \frac{\Gamma^2}{4}\hat{C}_{N-2}^2 \right)$$ \hfill (25)

where the tridiagonal and symmetric matrix $\hat{C}_N$ corresponds to the matrix $C_N$ for $\Gamma = 0$ (wire non coupled with electrodes) and $\hat{C}_N$ is the determinant of $C_N$. The above relations allows us to write the transmittance, Eq. 19, in the following form:

$$T(\epsilon) = \frac{\Gamma^2}{2|C_N|^2} \left\{ |\text{cof}(C_N)_{N,1}|^2 + \hat{C}_{N-1}^2 - \hat{C}_{N-2}\hat{C}_N \right\}$$ \hfill (26)

This relation is very important analytical relation obtained by means of the evolution operator method. Note, that the transmittance of $N$-site wire is expressed only by the tridiagonal matrix elements which can be obtained fully analytically. Note, that analytical calculations for the transmittance of a quantum wire, obtained by means of the evolution operator method, were not reported in literature (the set of differential equations for $U_{i,\vec{k}L}$ were solved numerically, e.g. [12]). In the next subsection we show that the above relation is equivalent to Eq. 14 obtained by means of the Green’s function technique.

### 3.3 Equivalence between EO and GF methods

In this part we show that using the special matrix relation which was introduced in Sec. 2, Eq. 2, we can transform the transmittance, Eq. 26 (evolution operator method), to Eq. 14 (Green’s function method). Note, that Eq. 26 for the transmittance seems very similar to Eq. 14 if only

$$\hat{C}_{N-1}^2 - \hat{C}_{N-2}\hat{C}_N = 0. \hfill (27)$$
But in general, this equivalence does not occur and one should obtain the appropriate determinants more carefully.

It is worth noting that the matrix $C_N$ has only two complex elements i.e. $(1,1)$ and $(N,N)$ elements, and the cofactor, $\text{cof}(C_N)_{N,1}$, is real. It means that the square of the absolute value for this cofactor is the same as the real square, i.e. $|\text{cof}(C_N)_{N,1}|^2 = [\text{cof}(C_N)_{N,1}]^2$. Now, using Eq. 2 the transmittance, Eq. 26 is expressed in the following form:

$$T(\varepsilon) = \Gamma^2 \frac{|\text{cof}(C_N)_{N,1}|^2}{|C_N|^2}$$  \hspace{1cm} (28)

The above result for the transmittance, Eq. 28 is the same as that one obtained by means of the retarded Green’s function, Eq. 14.

### 4 Conclusions

In this paper the analytical formula for the transmittance through a quantum wire has been obtained by means of the evolution operator technique, Eq. 26. In our calculation the set of differential equations, Eq. 20 has been resolved and helpful relation on tridiagonal matrixes has been used, Eq. 2. The transmittance, Eq. 26 has been transformed to well known in the literature relation obtained by means of the retarded Green’s function technique, Eq. 14. Our analytical calculations are not trivial and can be helpful in many physical phenomena where tridiagonal matrices appear. It is worth noting that the evolution operator method can be used also to describe time-dependent phenomena in nanostructures like e.g. photon assisted tunnelling in quantum wires [12], driven quantum dot systems [11], chemisorption processes or collision of atoms with a metallic surface [13, 14], decoherence processes in qubits and many others.

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