Some linear differential expressions for an electron scattering problem in a field of the one-dimensional arbitrary potential

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Abstract

The linear system of differential equations for determination of transmission and reflection amplitudes of scattered electron in the field of one dimensional arbitrary potential is obtained. It is shown that in general the scattering problem can be reduced to the Caushy problem for the stationary Shrodinger equation. An explicit functional for a dependance of transmission amplitude from scattered field is found.
I. Introduction

There have been many studies for investigation quantum particle propagation in the one-dimensional nonregular systems. It is well known that this problem has approaches in many fields of physics, particularly, it has important role for the transport theory of different perturbations in the linear quaziperiodical, disordered and random systems. An electron scattering problem in the field of the one-dimensional arbitrary potential is one of the key problem of such theories. Therefore to have a method for calculation transmission amplitude (TA) and reflection amplitude (RA) of an electron for one-dimensional arbitrary shape potential is actual.

This problem is the problem which is included in quantum mechanics textbooks. It is well known that the problem of determination TA and RA is reduced to the solution of the Shrodinger equation for wave function ($\hbar^2 = 2m_0 = 1$)

$$\frac{d^2\Psi}{dx^2} + (E - V(x))\Psi = 0$$  \(1\)

Here $V(x)$ is an arbitrary limited function which tends to zero, when $x \to \pm \infty$.

Asymptotic behavior of the solution for $\Psi$ is written in the form of

$$\Psi(x) = e^{ik_0 x} + Re^{-ik_0 x}, \text{ when } x \to -\infty, \hspace{1cm} (2)$$

$$\Psi(x) = Te^{ik_0 x}, \text{ when } x \to +\infty, \hspace{1cm} (3)$$

where $T$ and $R$ are electron TA and RA for potential $V(x)$ and $k_0 = \sqrt{E}$. In this approach to find $T$ and $R$ one have to solve the wave equation (1) with conditions (2),(3).

Using the phase function method one can directly calculate $T$ and $R$ \[2,3\] In this method scattering amplitudes are considered as a function of coordinate $x$, so that $T(x)$ and $R(x)$ correspond to TA and RA for the part of potential closed in the interval $(x, +\infty)$. Then, for functions $T(x)$ and $R(x)$ it was obtained a system of nonlinear equations. Particularly, the equation for RA is an ordinary Recatty equation:

$$\frac{dR(x)}{dx} = \frac{iV(x)}{2k_0} (e^{ik_0 x} + Re^{-ik_0 x})^2,$$  \(4\)
\[ R(\infty) = 0, \]

where \( R(x) \) is RA for potential

\[ U(x) = V(x')\theta(x - x'), \quad (5) \]

\( \theta(x) \) is step function. The equation (4) is well studied, but its analytical solution for given potential is not always known.

The aim of this paper’s to show, that in contrast to (4), with the help of convenient choice of unknown function as a combination \( T(x) \) and \( R(x) \), the problem of determination \( T_A \) and \( R_A \) is reduced to the problem of solution of the system of linear differential equations. We obtained this result from the consideration of the problem of an electron propagation in the one-dimensional chain with potential

\[ V(x) = \sum_{n=1}^{N} V_n(x - x_n), \quad (6) \]

where \( V(x - x_n) \) is an individual potential of the chain located near the point \( x_n \). It is suggested as well, that individual potentials do not have general points. Using the linear recurrent expressions for \( T_A \) and \( R_A \) for potential (4) and approximating an arbitrary function with the help of rectangular potentials, we obtain the linear differential equations for determination \( T \) and \( R \).

Some results of this work connected to the plane wave propagation through one-dimensional arbitrary linear medium were published in the paper.

This work consist from 7 sections. In (Sec. 2) the recurrent equations for \( T_A \) and \( R_A \) in one-dimensional chain is found. In (Sec. 3) the system of lineal differential equations for determination scattering amplitudes for a potential of an arbitrary shape is obtained. Further, in (Sec. 4) we show that the scattering problem can be formulated as a Caushy problem for Schroedinger equation. In (Sec. 5) the explicit functional for \( T_A \) from scattered potential is found. In conclusion the advantage and connection of suggested method to well known approach are discussed.
II. Recurrent relations for $T_N$ and $R_N$

Let us consider the problem of determination of transmission amplitude $T_N$ and reflection amplitude $R_N$ for the potential (3). It is well known that this problem is reduced to calculation of the $N$ matrixes product $^{5,6}$:

$$
\begin{pmatrix}
T_N \\
R_N
\end{pmatrix}
= \prod_{N}^{n=1}
\begin{pmatrix}
1/t_n^{*} & -r_n^{*}/t_n^{*} \\
-\frac{r_n}{t_n} & 1/t_n \\
\end{pmatrix}
\begin{pmatrix}
1 \\
R_N
\end{pmatrix},
$$

(7)

where $t_n$ and $r_n$ are TA and RA of the individual potential $V_n(x-x_n)$. When $V_n(x-x_n)$ are rectangular potentials with arbitrary widths $d_n$ and magnitudes of potential $V_n$, the scattering amplitudes $t_n$ and $r_n$ are given by the well known formulas $^{7}$:

$$
t_{n-1}^{-1} = \exp i k_0 d_n \left\{ \cos k_n d_n - i \frac{k_n^2 + k_0^2}{2k_n k_0} \sin k_n d_n \right\},
$$

(8)

$$
r_n/t_n = i \exp 2k_0 x_n \frac{k_n^2 - k_0^2}{2k_n k_0} \sin k_n d_n.
$$

(9)

where $k_n = \sqrt{E - V_n}$, $x_n$ is a coordinate of the middle point of the potential.

Let us show, that the problem of calculation of the $N$-th two-order matrixes product (7) is equivalent to solution of some linear recurrent equation. Let us denote

$$
\begin{pmatrix}
1/T_{N-1} \\
-R_{N-1}/T_{N-1}
\end{pmatrix}
= \prod_{N=1}^{2}
\begin{pmatrix}
1/t_n^{*} & -r_n^{*}/t_n^{*} \\
-\frac{r_n}{t_n} & 1/t_n \\
\end{pmatrix},
$$

(10)

then, as it is clear from (10), $T_{N-1}$ and $R_{N-1}$ are TA and RA of potential (4) in which the first th and $N$th individual potentials are absent.

From (3) and (10) for quantities $S_N = 1/T_N$ and $\bar{S}_N = R_N/T_N$ the following recurrent relations can be obtained;

$$
S_N = 1/t_N t_1 S_{N-1} + r_N r_1^{*}/t_N t_1^{*} S_{N-1} + r_1^{*}/t_N t_1 \bar{S}_{N-1} + r_N/t_N t_1 \bar{S}_{N-1},
$$

(11)

$$
\bar{S}_N = 1/t_N t_1^{*} \bar{S}_{N-1} + r_N r_1/t_N t_1 \bar{S}_{N-1} + r_1/t_N t_1 S_{N-1} + r_N/t_N t_1^{*} S_{N-1}.
$$

(12)

The recurrent equations (11), (12) will be used to solve the problem (3)-(4) for an arbitrary potential $V(x)$. 

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III. The system of linear differential equations for $T(x_1, x_2)$ and $R(x_1, x_2)$

Let us introduce functions $S(x_1, x_2) = 1/T(x_1, x_2)$ and $\overline{S}(x_1, x_2) = R(x_1, x_2)/T(x_1, x_2)$, where $T(x_1, x_2)$ and $R(x_1, x_2)$ are TA and RA for the part of potential $V(x)$, which is included between the points $x_1$ and $x_2$, so if $x_1 < x_2$ we have

$$U(x, x_1, x_2) = V(x)\theta(x - x_1)\theta(x_2 - x), \quad (13)$$

Then the function $U(x, x_1 - \Delta x_1, x_2 + \Delta x_2)$, when $\Delta x_1$ and $\Delta x_2$ are small enough, can be represented as the function $U(x, x_1, x_2)$ with two rectangular potentials added to it. One of the rectangular potentials added to the left side will be characterized by the value of potential $V(x_1)$ and the width $\Delta x_1$, second one added to the right side will be characterized by the value of potential $V(x_2)$ and the width $\Delta x_2$.

From (8), (9) for TA and RA for infinitely narrow rectangular potential ($d_n << 1$) we have

$$t_n^{-1} = 1 + \frac{iV_n d_n}{2k_0}, \quad r_n/t_n = -\frac{iV_n d_n}{2k_0} \exp{2ik_0x}, \quad (14)$$

Let us substitute in (11), (12) $S_N$ as $S(x_1 - \Delta x_1, x_2 + \Delta x_2)$ and $\overline{S}_N$ as $\overline{S}(x_1 - \Delta x_1, x_2 + \Delta x_2)$, $S_{N-1}$ as $S(x_1, x_2)$, $\overline{S}_{N-1}$ as $\overline{S}(x_1, x_2)$ and expand the obtained expressions in a series in infinitely small quantities $\Delta x_1, \Delta x_2$. Then, taking into account (14), it is possible to obtain the system of following linear differential equations:

$$\frac{\partial S}{\partial x_1} = -\frac{iV(x_1)}{2k_0}S - \frac{iV(x_1)}{2k_0} \exp\{-2ik_0x\}\overline{S}, \quad (15)$$

$$\frac{\partial \overline{S}}{\partial x_1} = \frac{iV(x_1)}{2k_0}\overline{S} + \frac{iV(x_1)}{2k_0} \exp\{2ik_0x\}S, \quad (16)$$

$$\frac{\partial S}{\partial x_2} = \frac{iV(x_2)}{2k_0}S - \frac{iV(x_2)}{2k_0} \exp\{2ik_0x\}\overline{S}, \quad (17)$$

$$\frac{\partial \overline{S}}{\partial x_2} = \frac{iV(x_2)}{2k_0}\overline{S} - \frac{iV(x_2)}{2k_0} \exp\{2ik_0x\}S, \quad (18)$$
The solutions of the system (15)-(18) have to be satisfied the following initial conditions

\[
S(x_1, x_2)|_{x_1=x_2} = 1, \quad \overline{S}(x_1, x_2)|_{x_1=x_2} = 0
\]  \hspace{1cm} (19)

Let us now show that the law of current density conservation follows from (15)-(18):

\[
|S(x_1, x_2)|^2 - |\overline{S}(x_1, x_2)|^2 = |T(x_1, x_2)|^2 + |R(x_1, x_2)|^2 = 1
\]  \hspace{1cm} (20)

for any \(x_1\) and \(x_2\). Differentiating (20) on \(x_1\) and \(x_2\) we get

\[
S^* \frac{\partial S}{\partial x_1} + S \frac{\partial S^*}{\partial x_1} - \overline{S} \frac{\partial \overline{S}}{\partial x_1} - \overline{S} \frac{\partial \overline{S}^*}{\partial x_1} = 0
\]  \hspace{1cm} (21)

\[
S^* \frac{\partial S}{\partial x_2} + S \frac{\partial S^*}{\partial x_2} - \overline{S} \frac{\partial \overline{S}}{\partial x_2} - \overline{S} \frac{\partial \overline{S}^*}{\partial x_2} = 0
\]  \hspace{1cm} (22)

Using equations (15)-(18) and (21),(22) it is easy to see the correctness of condition (20).

Let us consider (15),(16) for fixed \(x_2\) and variable \(x_1\). Denoting \(S(x_1, x_2) \equiv P(x)\) and \(\overline{S}(x_1, x_2) \equiv \overline{P}(x)\) for functions \(P(x)\) and \(\overline{P}(x)\) the following differential equations are obtained;

\[
\frac{dP}{dx} = -\frac{iV(x)}{2k_0} P - \frac{iV(x)}{2k_0} \exp\{-2ik_0x\} \overline{P}, \hspace{1cm} (23)
\]

\[
\frac{d\overline{P}}{dx} = \frac{iV(x)}{2k_0} P + \frac{iV(x)}{2k_0} \exp\{2ik_0x\} P, \hspace{1cm} (24)
\]

The initial conditions for (23)-(24) are

\[
P(\infty) = 1 \text{ and } \overline{P}(\infty) = 0
\]  \hspace{1cm} (25)

The equations (23)-(24) describe the dependance of scattering parameters \(T(x)\) and \(R(x)\) on \(x\) for potential

\[
U(x) = V(y)\theta(x - y).
\]

In the case of the fixed \(x_1\) and variable \(x_2\) for the functions \(S(x_1, x_2) \equiv D(x)\) and \(\overline{S}(x_1, x_2) \equiv \overline{D}(x)\) the following equations are obtained from (17),(18):
\[ \frac{dD}{dx} = \frac{iV(x)}{2k_0} D - \frac{iV(x)}{2k_0} \exp\{2ik_0x\} \overline{D}, \quad (26) \]

\[ \frac{d\overline{D}}{dx} = -\frac{iV(x)}{2k_0} \overline{D} + \frac{iV(x)}{2k_0} \exp\{-2ik_0x\} D \quad (27) \]

The initial conditions for (26),(27) are

\[ D(-\infty) = 1 \text{ and } \overline{D}(-\infty) = 0 \quad (28) \]

The equations (26),(27) describe the dependence of scattering parameters \( T(x) \) and \( R(x) \) on \( x \) for the potential

\[ U(x) = V(y)\theta(y - x) \]

So the problem of the determination \( T \) and \( R \) is reduced in general to the problem of solution of the system differential equations (23)-(24) or (26),(27) with initial conditions (25) or (28).

**IV. The problem of a Cauchy for a scattering parameters.**

In this section we will show that, using equations (23),(24) or (26),(27) it is possible to get the two linear equations for combinations of functions \( P(x) \), \( \overline{P}(x) \) or \( D(x) \), \( \overline{D}(x) \), one of which is the Schrödinger equation, another one is the primary first order differential equation. Let us present (23)-(24) in the following form:

\[ \exp\{ik_0x\} \frac{dP}{dx} = -\frac{iV(x)}{2k_0} \left[ P \exp\{ik_0x\} + \overline{P} \exp\{-ik_0x\} \right], \quad (29) \]

\[ \exp\{-ik_0x\} \frac{d\overline{P}}{dx} = \frac{iV(x)}{2k_0} \left[ P \exp\{ik_0x\} + \overline{P} \exp\{-ik_0x\} \right]. \quad (30) \]

Let us introduce the functions \( F_1 \) and \( \overline{F}_1 \):

\[ P \exp\{ik_0x\} = F_1 \text{ and } \overline{P} \exp\{-ik_0x\} = \overline{F}_1 \quad (31) \]
and write (29)-(30) in the form of
\[
\frac{dF_1}{dx} - ik_0 F_1 = -i \frac{V}{2k_0} \{ F_1 + \overline{F}_1 \}, \tag{32}
\]
\[
\frac{dF_1}{dx} + ik_0 F_1 = i \frac{V}{2k_0} \{ F_1 + \overline{F}_1 \}. \tag{33}
\]

From these equations it is easy to show that for quantities \( F_1 + \overline{F}_1 = L_1 \) and \( F_1 - \overline{F}_1 = Q_1 \) we have equations
\[
\left[ \frac{d^2}{dx^2} + E - V(x) \right] L_1(x) = 0, \quad Q_1 = -i \frac{dL_1}{k_0 dx}. \tag{34}
\]

Introducing quantities \( D \exp\{-ik_0 x\} = F_2 \) and \( D \exp\{ik_0 x\} = \overline{F}_2 \), and using equations (23)-(27) for the functions \( F_2 - \overline{F}_2 = L_2 \) and \( F_2 + \overline{F}_2 = Q_2 \) the following equations are received:
\[
\frac{d}{dx} Q_2 = -\frac{i}{k_0} \left( k_0^2 - V(x) \right) L_2, \tag{35}
\]
\[
\frac{dL_2}{dx} = -ik_0 Q_2. \tag{36}
\]

Excluding the function \( Q_2 \) from equation (35), we get
\[
\left[ \frac{d^2}{dx^2} + E - V(x) \right] L_2(x) = 0, \quad Q_2 = i \frac{dL_2}{k_0 dx}. \tag{37}
\]

Let us now apply the equation (37) to the problem of determination of TA and RA for an arbitrary potential \( V(x) \) with finite size (the potential \( V(x) \) equals to zero outside of some interval \( a \leq x \leq b \)).

Inserting \( L_2 \equiv L, \ F_2 \equiv F \) and \( \overline{F}_2 \equiv \overline{F} \), then from (37) we get
\[
F = \frac{1}{2} \left( \frac{i}{k_0} \frac{dL}{dx} + L \right), \quad \overline{F} = \frac{1}{2} \left( \frac{i}{k_0} \frac{dL}{dx} - L \right) \tag{38}
\]
and
\[
\left[ \frac{d^2}{dx^2} + E - V(x) \right] L(x) = 0. \tag{39}
\]
The boundary conditions for function $L(x)$ at the point $x = a$ are

$$L(a) = \exp\{-ik_0 a\}, \quad (dL/dx)|_{x=a} = -ik_0 \exp\{-ik_0 a\}. \quad (40)$$

Let us seek solution of (39) in the form

$$L(x) = \exp\{-ik_0 a\} \left( H_1(x) - ik_0 H_2(x) \right). \quad (41)$$

Then the real functions $H_1$ and $H_2$ satisfy the equation (39) with boundary conditions

$$H_1(a) = 1, \quad (dH_1/dx)|_{x=a} = 0 \quad and \quad H_2(a) = 0, \quad (dH_2/dx)|_{x=a} = 1. \quad (42)$$

Substituting the solution (41) into (38) and taking into account the connection between $F$, $\overline{F}$ and $D$, $\overline{D}$ we obtain

$$\frac{1}{T} = \frac{1}{2} \exp\{i k_0 d\} \left[ H_1 + \frac{dH_2}{dx} - ik_0 H_2 + \frac{i}{k_0} \frac{dH_1}{dx} \right], \quad (43)$$

$$\frac{R}{T} = \frac{1}{2} \exp\{i 2 k_0 x_0\} \left[ -H_1 + \frac{dH_2}{dx} - ik_0 H_2 - \frac{i}{k_0} \frac{dH_1}{dx} \right], \quad (44)$$

where $x_0 = (b + a)/2$ and $d = b - a$.

Thus, we showed, that the solution of the problem (1)-(3), i.e. the problem of determination RA and TA for an arbitrary potential, is reduced to a Cauchy problem for the Schrödinger equation (39).

In the end of this section, using equations (35), (36), we will bring the differential equations for the transmission coefficient $|T|^2 = |D|^2$ and reflection coefficient $|R|^2 = |\overline{D}|^2 / |D|^2$. The result which we obtained can be represented in the following way. If the unknown functions $|D|^2$ and $|\overline{D}|^2$ are expressed by the function $M$ as

$$|D|^2 = \frac{1}{2} \left( \frac{M}{2 k_0^2} + 1 \right), \quad |\overline{D}|^2 = \frac{1}{2} \left( \frac{M}{2 k_0^2} - 1 \right), \quad (45)$$

then the function $M(x)$ are connected with the function $G(x)$ by differential equation:

$$\frac{dM}{dx} = V(x) \frac{dG}{dx}, \quad (46)$$
and function $G(x)$ is the solution of the equation:

$$\frac{d^3 G}{dx^3} + 4(E - V(x)) \frac{dG}{dx} - 2\frac{dV}{dx} G = 0,$$

with initial conditions

$$G(a) = 1, \quad (dG/dx)|_{x=a} = 0, \quad (d^2 G/dx^2)|_{x=a} = 2V(a).$$

V. Functional $T[V(x)]$

In this section we bring an explicit form of the functional $T[V(x)]$. To do it, let us assume that in (11) and (12) $t_1 = 0, \ r_1 = 1$. It means, that we add an rectangular potential only from the right hand side of the chain. For this case, inserting $S_N \equiv D_N$, $S_N^* \equiv D_N^*$, one can write (11), (12) in the form

$$D_N = \frac{r_N}{t_N} D_{N-1} + \frac{1}{t_N} D_{N-1},$$

$$D_N^* = \frac{r_N^*}{t_N^*} D_{N-1} + \frac{1}{t_N^*} D_{N-1}.$$  

Note, that here $N$ is a variable. Let us represent (43), (44) in a more convenient form. Excluding $D_{N-1}$ from the first equation and $D_{N-1}$ from the second one, we get two independent equations for $D_N$ and $D_N^*$:

$$D_N = A_N D_{N-1} - B_N D_{N-2}, \ N \geq 2$$

$$D_N^* = A_N^* D_{N-1}^* - B_N^* D_{N-2}^*, \ N \geq 2$$

where $A_N = \frac{1}{t_N} + \frac{B_N}{t_N^* - t_{N-1}}$ and $B_N = r_N t_N / t_N r_N$.

Let us apply the obtained result (51) for the potential consisted from infinitely narrow rectangular potentials (14). In this case $A_N$ and $B_N$ are

$$A_N = 1 + B_N + \frac{i V_N d_N}{2k_0} \left[ 1 - \exp\{i2k_0(x_N - x_{N-1})\} \right],$$

$$B_N = \frac{V_N d_N}{V_{N-1} d_{N-1}} \exp\{i2k_0(x_N - x_{N-1})\}.$$
Representing $D_N$ in the form

$$D_N = 1 + \sigma_N + \sigma_{N-1} + \cdots + \sigma_1,$$  \hspace{1cm} (55)

where

$$\sigma_N = \frac{iV_N d_N}{2k_0} \{1 + f_{N,N-1} \sigma_{N-1} + f_{N,N-2} \sigma_{N-2} + \cdots + f_{N,1} \sigma_1\}$$

and $f_{N,n} = \exp\{i2k_0(x_N - x_n)\}$, $\sigma_1 = \frac{iV_1 d_1}{2k_0}$, for $D_N = T_N^{-1}$ the following expression is found

$$T_N^{-1} = 1 + \sum_{p=1}^{N} \sum_{1 \leq n_1 < \cdots < n_p} \frac{iV_{n_1} d_{n_1}}{2k_0} \cdots \frac{iV_{n_p} d_{n_p}}{2k_0} \prod_{l=1}^{p-1} \left[1 - \exp\{i2k_0(x_{n_{l+1}} - x_{n_l})\}\right].$$ \hspace{1cm} (56)

Putting $V_n$ as $V(x_n)$ and tending $N \to \infty$ and $\max d_n \to 0$ it is possible from (56) to obtain the following series:

$$T^{-1} = 1 + \sum_{n=1}^{\infty} W_n,$$ \hspace{1cm} (57)

where

$$W_n = \int_{x_{n-1}}^{x_{n-1}} \int_{x_{n-2}}^{x_{n-2}} \cdots \int_{x_{n-1}}^{x_{n-1}} \frac{iV(x_1)}{2k_0} \cdots \frac{iV(x_n)}{2k_0} \prod_{l=1}^{n-1} \left[1 - \exp\{i2k_0(x_{l+1} - x_l)\}\right] dx_1 \cdots dx_n$$ \hspace{1cm} (58)

The expression (57) are the explicit expression for functional $T[V(x)]$.

VI. Conclusion

The important result of this work is the suggestion, that for scattering problem instead of solving the Srodinger equation for $\Psi$ (1)-(3), we can consider the system of linear equations for $T^{-1}$ and $R/T$, i.e. to consider equations (23), (24) or (26), (27).

Particularly, from these equations one can derivide the Recatty equation (4), for $R(x)$. This equation nonlinear and its analytical solutions are known for a limited class of potentials.
Here we have shown that the problem of determination of the functions $T(x)$ and $R(x)$ is reduced to solution of the linear equation for function $L$, which is some given combination from $T(x)$ and $R(x)$. It is important to note, that this equation coincides with the well studied Srodinger equation.

The another important result is the differential equations for transmission and reflection coefficients for an arbitrary potentials $V(x)$. Since the value of function $G$ and their derivations are known in the initial point of the potential, the problem can be formulated as Caussy problem.

Supposing, that potential $V(x) = const$, when $a \leq x \leq b$ and $V(x) = 0$, when $x < a, x > b$, the well known result for transmission coefficient for rectangular one can obtain from (45)-(48). Indeed, solving equations (46)-(48) when $V(x) = V_0$, for function $M(x)$ we get

$$M^2 = \frac{V_0^2}{2k_0^2} \sin^2 kx + 1.$$  \hspace{1cm} (59)

Putting (59) in (45) we obtain the following expression for transmission coefficient of the rectangular potential

$$|T|^2 = \frac{4k_0^2k^2}{(k_0^2 - k^2)^2 \sin^2 kx + 4k_0^2k^2}$$  \hspace{1cm} (60)

where $k = \sqrt{E - V_0}$.

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