An application of a quantum wave impedance approach for solving a nonsymmetric single well problem

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Abstract

A short introduction of a relation between a Green’s function and a quantum wave impedance function as well as its application to a determination of eigenenergies and eigenfunctions of a quantum-mechanical system is provided. Three different approaches, namely a classical approach based on a direct solving of a Schrödinger equation, a transfer matrix method and a quantum wave impedance technique, for a calculation of eigenenergies and eigenfunctions of a quantum mechanical nonsymmetric single well system are considered. A comparison of these approaches gives the possibility to clarify advantages and drawbacks of each method which is useful especially for teaching and learning purposes.

1 Introduction

For the first time an introduction of a quantum wave impedance concept was done in 1988 by the authors of the pioneer article on this topic [1]. Accordingly to their statement the primary purpose of this article was to show that the well-developed theory of electrical transmission lines can be effectively used for calculating the quantum mechanical transmission probability. One year later the same authors have published an article [2] in which they calculated the traversal time of electrons in resonant tunnelling structures and showed that the real part of the quantum-mechanical wave impedance, at resonance, can be used to calculating
the electron traversal time. They concluded and emphasized the usefulness of a quantum-mechanical impedance concept and the simplicity of using the transmission line equation.

In many other papers [3, 4, 5, 6, 7, 8, 9, 10, 11, 12] the efficacy of a quantum wave impedance approach for an analysis of quantum-mechanical structures with a potential which has a complicated spatial structure was demonstrated but only in the paper [13] it was shown how on the base of a the Shrödinger equation to get an equation for a quantum wave impedance function and to reformulate the scattering and bound states problems in terms of a quantum wave impedance.

Despite the fact just mentioned the relation between a Green’s function and a quantum wave impedance function was established more quite long ago [5]. The approach of Green’s functions is very useful for solving non-homogeneous boundary value problems which is very close, from a mathematical point of view, to the main reason of a quantum wave impedance introduction.

A few years later in [14] a technique of a calculation of the normalized wave functions in arbitrary one-dimensional quantum well structures was described. Authors using the relation between Green’s function and a quantum wave impedance presented an efficient technique of calculating both the eigenenergies and the normalized eigenfunctions in quantum wells. This method is particularly attractive in numerical calculations of multibarrier devices in which the estimation of the self-consistent potential is desired. The method is computationally efficient and is generalized enough to model arbitrary wells under an applied bias voltage including the effects of space charge.

The aim of this article is to provide the comparison of a quantum wave impedance approach with a classical one (based on a direct solving of a Shrödinger equation) and with a transfer matrix method. We will apply mentioned approaches specifically for finding energies and wave functions of bound states. It will help one to clearly understand advantages and drawbacks of a quantum wave impedance method.

To fulfil our task we will consider very simple system. But it is enough to understand the main features of each approach. So, assume that we have a nonsymmetric rectangular potential well of a finite depth:

\[
U(x) = \begin{cases} 
U_1 > 0, & x \leq 0 \\
U_2 < 0, & 0 < x < a \\
U_3 > 0, & x > a
\end{cases}
\]  

We are going to find energies and wave functions of bound states and these states have an energy \( E < \max(U_1, U_3) \).
2 The relation between a Green’s function and a quantum wave impedance

The equation for a Green’s function $G(x, x', E)$ is as follows

\[
\left( E + \frac{\hbar^2}{2m} \frac{d^2}{dx^2} - U(x) \right) G(x, x', E) = \delta(x - x'). \tag{2}
\]

It coincides with the Shrödinger equation everywhere besides point $x = x'$ and this fact pushes us to introduce an extended quantum wave impedance function $\tilde{Z}(x, x')$ in the following way

\[
\tilde{Z}(x, x') = \frac{\hbar}{im} \frac{\partial G(x, x', E)}{\partial x}. \tag{3}
\]

Then on the base of the equation (2) we get

\[
\frac{d\tilde{Z}(x, x')}{dx} + i\frac{m}{\hbar} \tilde{Z}^2(x, x') = i \frac{2}{\hbar} (E - U(x)) - i \frac{2}{\hbar} \delta(x - x'). \tag{4}
\]

If $U(x)$ is not singular then after integration of both left and right sides of the previous equation we obtain:

\[
Z^+(x') - Z^-(x') = i \frac{2}{\hbar} G^{-1}(x', x', E) \tag{5}
\]

or

\[
G(x', x', E) = -i \frac{2}{\hbar} \frac{1}{Z^+(x') - Z^-(x')}. \tag{6}
\]

where

\[
Z^-(x') = \tilde{Z}(x' + 0, x'), \quad Z^+(x') = \tilde{Z}(x' - 0, x'). \tag{7}
\]

If we apply boundary conditions for $\tilde{Z}(x, x')$ at points with coordinates $a$ and $b$ then instead of $Z^-(x')$ and $Z^+(x')$ we can use $Z^-(x', b)$ and $Z^+(x', a)$, where $a < x' < b$. Notice that $Z^-(x', b)$ and $Z^+(x', a)$ are the same ones as in a 13. Now we can transit the well-know relations obtained within Green’s function approach to a formalism of a quantum wave impedance.

Now let’s consider the following relation:

\[
G(x, x', E + i\varepsilon) = \sum_m \frac{\psi_m(x)\psi_m^*(x')}{E - E_m + i\varepsilon}, \tag{8}
\]
where \( \varepsilon \to 0 \) and thus
\[
\lim_{E \to E_n} G(x, x, E + i\varepsilon) = \frac{|\psi_n(x)|^2}{E - E_n + i\varepsilon}.
\] (9)

Taking an imaginary part of both sides of the previous relation we get
\[
|\psi_n(x)|^2 = -\varepsilon \Im [G(x, x, E_n - i\varepsilon)]
\] (10)
or using a quantum wave impedance we obtain
\[
|\psi_n(x)|^2 = \frac{2\varepsilon}{\hbar} \Im \left( \frac{i}{Z^-(x, b, E_n - i\varepsilon) - Z^+(x, a, E_n - i\varepsilon)} \right).
\] (11)

3 Nonsymmetric well of a finite depth. Quantum wave impedance approach

Characteristic impedances for each region of a potential (1) are
\[
z_1 = \frac{\hbar \kappa_1}{m}, \quad z_2 = \frac{i k_2 a}{m}, \quad z_3 = \frac{\hbar \kappa_3}{m}.
\] The load impedance coincides with the characteristic impedance of a third region \( z_3 \). Calculating the input impedance at a point \( x = 0 \), on the base of a well-known formula [1], and equating it to \( -z_1 \) [13] we easily get the expression for determining energies of bound states:
\[
-z_1 = z_2^2 \frac{z_3 \cos[k_2 a] - z_2 \sin[k_2 a]}{z_2 \cos[k_2 a] - z_3 \sin[k_2 a]} = z_2 \frac{z_3 - z_2 \tan[k_2 a]}{z_2 - z_3 \tan[k_2 a]}
\] (12)
or reminding the relations between \( z_m \) and \( k_m \), \( m = 1, 2, 3 \) we obtain the same formula as in two previous sections
\[
\tan(k_2 a) = \frac{k_2 (z_1 + z_3)}{z_1 z_3 - k_2^2}.
\] (13)

It is easy to notice that a quantum wave impedance approach for the calculation of eigenenergies demands much less efforts than the classical method or a transfer matrix formalism.

To find wave functions of bound states in this system let’s find the values of \( Z^-(x, b; E) \) and \( Z^+(x, a; E) \) in the second region of a potential (1). It is easy to do [13] since that region has a constant value of a potential energy. Thus,

\[
Z^-(x, a; E) = z_2 \tan(ik_2 x + \phi_R),
\]
\[
Z^+(x, 0; E) = z_2 \tan(ik_2 x + \phi_L),
\] (14)

where
\[
\phi_R = -\frac{1}{2} \ln \left( \frac{\exp(2ik_2 a) \frac{z_2 - z_3}{z_2 + z_3}}{\frac{z_2}{z_2 + z_3}} \right) = -\frac{1}{2} \ln \left( \frac{\exp(2ik_2 a) k_2 - ik_3}{k_2 + ik_3} \right),
\]
\[
\phi_L = -\frac{1}{2} \ln \left( \frac{z_1 + z_2}{z_2 - z_1} \right) = -\frac{1}{2} \ln \left( \frac{ik_1 + k_2}{k_2 - ik_1} \right).
\] (15)
The Taylor series of $Z^+(x, 0; E_n - i\varepsilon)$ and $Z^-(x, a; E_n - i\varepsilon)$ have the following form

$$Z^-(x, a; E_n - i\varepsilon) = Z^+(x, E_n) + i \frac{\kappa_3 a + 1}{\kappa_3} \varepsilon + O(\varepsilon^2),$$

$$Z^+(x, 0; E_n - i\varepsilon) = Z^-(x, E_n) + i \frac{1}{\hbar \kappa_1} \varepsilon + O(\varepsilon^2),$$

where $E_n$ we find from the condition $\phi_L = \phi_R$ and it gives the same relation as we got in the previous sections. Now using the obtained earlier relation we finally get

$$|\psi_2(x)|^2 = 2 \left(a + \frac{\kappa_1 + \kappa_3}{\kappa_1 \kappa_3}\right)^{-1} \cos^2(k_2 a + \phi),$$

where $\phi \equiv \phi_L = \phi_R$.

4 Classical approach

Having the potential energy in a form we get the following Shrödinger equations in each region

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_1(x) + U_1 \psi_1(x) = E \psi_1(x), \quad x \leq 0,$$

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_2(x) + U_2 \psi_1(x) = E \psi_2(x), \quad 0 < x \leq a,$$

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_3(x) + U_3 \psi_1(x) = E \psi_3(x), \quad x > a.$$  

(18)

And general solutions of these equations (in each region) for an energy $E < \max(U_1, U_3)$ are easy enough

$$\psi_1(x) = C_{11} \exp(\kappa_1 x) + C_{12} \exp(-\kappa_1 x),$$

$$\psi_2(x) = C_{21} \cos(k_2 x) + C_{22} \sin(k_2 x),$$

$$\psi_3(x) = C_{31} \exp(\kappa_3 x) + C_{32} \exp(-\kappa_3 x),$$

(19)

where

$$\kappa_1 = \frac{\sqrt{2m(U_1 - E)}}{2m}, \quad k_2 = \frac{\sqrt{2m(E - U_2)}}{\hbar}, \quad \kappa_3 = \frac{\sqrt{2m(U_3 - E)}}{\hbar}.$$  

(20)

One also has to apply boundary and matching conditions:

$$\psi_1(-\infty) = 0, \quad \psi_1(0) = \psi_2(0),$$

$$\psi_1'(0) = \psi_2'(0), \quad \psi_2(0) = \psi_3(0),$$

$$\psi_2'(0) = \psi_3'(0), \quad \psi_3(\infty) = 0.$$  

(21)
The first condition and the last one lead to \( C_{12} = 0 \) and \( C_{31} = 0 \). The rest conditions give

\[
C_{11} = C_{21}, \quad C_{11} k_1 = C_{22} k_2,
\]

\[
C_{21} \cos(k_2 a) + C_{22} \sin(k_2 a) = C_{32} \exp(-k_3 a),
\]

\[
-C_{21} k_2 \sin(k_2 a) + C_{22} k_2 \cos(k_2 a) = -k_3 C_{32} \exp(-k_3 a)
\]

or

\[
k_2 \frac{\kappa_1 - k_2 \tan(k_2 a)}{k_2 + \kappa_1 \tan(k_2 a)} = -k_3,
\]

which finally gives the relation for a determination of energies of bound states

\[
\tan(k_2 a) = \frac{k_2 (\kappa_1 + \kappa_3)}{\kappa_3 - k_2^2}.
\]

To determine the wave functions of bound states in this system we depict it in the following form

\[
\psi(x) = \begin{cases} 
C_{11} \exp(\kappa_1 x), & x < 0 \\
C_{21} \cos(k_2 a) + C_{22} \sin(k_2 a), & 0 \leq x \leq 0 \\
C_{32} \exp(-\kappa_3 x), & x > a
\end{cases}
\]

To find constants \( C_{11}, C_{21}, C_{22}, C_{32} \) we have to solve the following matrix equation:

\[
\begin{pmatrix}
1 & -1 & 0 & 0 \\
\kappa_1 & 0 & -k_2 & 0 \\
0 & \cos(k_2 a) & \sin(k_2 a) & -e^{-\kappa_3 a} \\
0 & -k_2 \sin(k_2 a) & k_2 \cos(k_2 a) & \kappa_3 e^{-\kappa_3 a}
\end{pmatrix}
\begin{pmatrix}
C_{11} \\
C_{21} \\
C_{22} \\
C_{32}
\end{pmatrix}
= \begin{pmatrix}
0 \\
0 \\
0 \\
0
\end{pmatrix}
\]

The existence of a non-trivial solution of this system of equations demands the determinant of this 4 \( \times \) 4 matrix to be equal to zero which bears the well-known relation (24). But it also means that values \( C_{11}, C_{21}, C_{22}, C_{32} \) are not independent and three of them (for example \( C_{21}, C_{22}, C_{32} \)) can be expressed through the other one (\( C_{11} \)):

\[
C_{21} = C_{11}, \quad C_{22} = \frac{\kappa_1}{k_2} C_{11},
\]

\[
C_{32} = C_{11} \exp(\kappa_3 a) \left\{ \cos(k_2 a) + \frac{\kappa_1}{k_2} \sin(k_2 a) \right\}.
\]

The final step is to determine \( C_{11} \). One can do it using the normalization condition for a
wave function of a bound state:

\[ |C_{11}|^2 \left( \int_{-\infty}^{0} \exp[2\kappa_1 x] dx + \int_{0}^{a} \left[ \cos(k_2 x) + \frac{\kappa_1}{k_2} \sin(k_2 x) \right]^2 dx \right. \]

\[ \left. + \exp(2\kappa_3 a) \left[ \cos(k_2 a) + \frac{\kappa_1}{k_2} \sin(k_2 a) \right]^2 \int_{a}^{\infty} \exp[-2\kappa_3 x] dx \right) = 1. \]  

(28)

After an integration we get

\[ \frac{1}{2\kappa_1} + \frac{1}{4k_2} \left( 1 - \frac{\kappa_1^2}{k_2^2} \right) \sin[2k_2 a] - \frac{\kappa_1}{2k_2} \cos[2k_2 a] + \]  

\[ + \frac{1}{2} \left( a + \frac{\kappa_1^2 a}{k_2^2} + \frac{\kappa_1}{k_2} \right) + \frac{1}{2k_3} \left[ \cos(k_2 a) + \frac{\kappa_1}{k_2} \sin(k_2 a) \right]^2 = \frac{1}{|C_{11}|^2}. \]  

(29)

On the base of both a relation \[24\] and the following formulas:

\[ \sin(2k_2 a) = \frac{2 \tan(k_2 a)}{\tan^2(k_2 a) + 1} = -\frac{2k_2(\kappa_1 \kappa_3 - k_2^2)(\kappa_1 + \kappa_3)}{(\kappa_1^2 k_2^2 + \kappa_3^2 k_2^2 + k_2^4 + k_2^2 \kappa_3^2)}, \]

\[ \cos(2k_2 a) = \frac{1 - \tan^2(k_2 a)}{\tan^2(k_2 a) + 1} = \frac{\kappa_2^2 k_2^2 - \kappa_1^2 \kappa_3^2 + 4 \kappa_1 \kappa_2 \kappa_3 - k_2^4 + k_2^2 \kappa_3^2}{\kappa_1^2 k_2^2 + \kappa_3^2 k_2^2 + k_2^4 + k_2^2 \kappa_3^2} \]  

(30)

one can transform the relation \[24\] to the following form

\[ |C_{11}|^{-2} = \frac{1}{2} \left( 1 + \frac{\kappa_1^2}{k_2^2} \right) \left( a + \frac{\kappa_1 + \kappa_3}{\kappa_1 \kappa_3} \right). \]  

(31)

It gives us the final expression for the square of a modulus of a wave function in the well \((0 < x < a)\):

\[ |\psi_2(x)|^2 = 2 \left( 1 + \frac{\kappa_1^2}{k_2^2} \right)^{-1} \left( a + \frac{\kappa_1 + \kappa_3}{\kappa_1 \kappa_3} \right)^{-1} \left( \cos(k_2 x) + \frac{\kappa_1}{k_2} \sin(k_2 x) \right)^2 = \]

\[ = \left( a + \frac{\kappa_1 + \kappa_3}{\kappa_1 \kappa_3} \right)^{-1} \left( \frac{\cos(k_2 a)}{\sqrt{1 + \frac{\kappa_1^2}{k_2^2}}} - \frac{-\kappa_1 / k_2 \sin(k_2 a)}{\sqrt{1 + \frac{\kappa_1^2}{k_2^2}}} \right)^2 = \]

\[ = \left( a + \frac{\kappa_1 + \kappa_3}{\kappa_1 \kappa_3} \right)^{-1} \cos^2(k_2 x + \phi), \]  

(32)

where

\[ \cos(\phi) = \frac{1}{\sqrt{1 + \frac{\kappa_1^2}{k_2^2}}}, \quad \sin(\phi) = -\frac{\kappa_1 / k_2}{\sqrt{1 + \frac{\kappa_1^2}{k_2^2}}}, \]  

(33)
5 Transfer matrix approach

To apply the transfer matrix approach we have to build three matrices and then to multiply them. The first matrix $I_{12}$ describes a wave transition through the interface ($x = 0$) between the first and the second region of a potential (1):

$$I_{12} = \frac{1}{2} \begin{pmatrix} \frac{\kappa_1 + ik_2}{\kappa_2} & \frac{ik_2 - \kappa_1}{\kappa_2} \\ \frac{ik_2 - \kappa_1}{\kappa_2} & \frac{\kappa_1 + ik_2}{\kappa_2} \end{pmatrix}. \quad (34)$$

A wave transferring inside the second region of a potential (1) is described by a second matrix, namely matrix $M$:

$$M = \begin{pmatrix} e^{ik_2 a} & 0 \\ 0 & e^{-ik_2 a} \end{pmatrix}. \quad (35)$$

And finally the transition through the interface ($x = a$) between a second and a third region of a potential (1) is described by a matrix $I_{23}$:

$$I_{23} = \frac{1}{2} \begin{pmatrix} \frac{\kappa_3 - ik_3}{\kappa_2} & \frac{\kappa_3 + ik_3}{\kappa_2} \\ \frac{\kappa_3 + ik_3}{\kappa_2} & \frac{\kappa_3 - ik_3}{\kappa_2} \end{pmatrix}. \quad (36)$$

Thus, the full transfer matrix has the following form

$$T = I_{12} M I_{23} = \frac{1}{4} \begin{pmatrix} \frac{\kappa_1 + ik_2}{\kappa_2} & \frac{ik_2 - \kappa_1}{\kappa_2} \\ \frac{ik_2 - \kappa_1}{\kappa_2} & \frac{\kappa_1 + ik_2}{\kappa_2} \end{pmatrix} \begin{pmatrix} e^{ik_2 a} & 0 \\ 0 & e^{-ik_2 a} \end{pmatrix} \begin{pmatrix} \frac{\kappa_3 - ik_3}{\kappa_2} & \frac{\kappa_3 + ik_3}{\kappa_2} \\ \frac{\kappa_3 + ik_3}{\kappa_2} & \frac{\kappa_3 - ik_3}{\kappa_2} \end{pmatrix} =$$

$$= \frac{k_2 (\kappa_1 + \kappa_3) \cos(k_2 a) + (\kappa_1 \kappa_3 - k_2^2) \sin(k_2 a)}{2k_2 \kappa_3}$$

$$\frac{k_2 (\kappa_3 - \kappa_1) \cos(k_2 a) - (\kappa_1 \kappa_3 + k_2^2) \sin(k_2 a)}{2k_2 \kappa_3}.$$ \quad (37)

The relation for a determination of energies of bound states is $M_{11} = 0$ or in the explicit form

$$\frac{k_2 (\kappa_1 + \kappa_3) \cos(k_2 a) + (\kappa_1 \kappa_3 - k_2^2) \sin(k_2 a)}{2k_2 \kappa_3} = 0,$$ \quad (38)

which gives the same expression as in the previous section

$$\tan(k_2 a) = \frac{k_2 (\kappa_1 + \kappa_3)}{\kappa_1 \kappa_3 - k_2^2}. \quad (39)$$

6 Conclusions

Making comparison of three different approaches which were described in this paper we can conclude that a quantum wave impedance approach for a calculation of energies of
bound states and their wave functions demands much less efforts than a classical method or a transfer matrix technique. Thus a quantum wave impedance approach is a powerful method for studying quantum mechanical systems and, in particular, can be applied for nanosystems with a complicated geometry of a potential energy. But it is also an elegant teaching and learning tool since it has quite simple both a physical interpretation and a mathematical technique.

It is worth to say that the paper [15] is dedicated to the similar problem, namely to the comparative analysis of traditional and impedance approaches in a modelling asymmetric potential quantum-mechanical barrier. As a result the authors stated that “impedance method significantly simplifies modelling of quantum-mechanical structures in comparison with the traditional method of solving quantum-mechanical problems”. But that paper does not consider nor a transfer matrix approach nor finding wave functions of bound states. This task we realized in this paper with hope that it will demonstrate other sides of a quantum wave impedance approach and its advantages.

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