Physica E 64 (2014) 141–145

Contents lists available at ScienceDirect

Physica E

journal homepage: www.elsevier.com/locate/physe

Connection between bound state and tunneling problems

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HIGHLIGHTS

- This paper shows the connection between bound states and tunneling problems.
- The transfer matrix is used to describe the bound state and tunneling problems.
- The approach can easily be taught in an introductory class in quantum mechanics.

ARTICLE INFO

Article history:
Received 15 May 2014
Received in revised form
14 July 2014
Accepted 17 July 2014
Available online 26 July 2014

Keywords:
Tunneling
Bound state energy level
Resonance
Transfer matrix

ABSTRACT

The transfer matrix formalism is used to show that the problem of finding the bound states of a quantum well with an arbitrary one-dimensional potential energy profile $E_c(x)$ can be reformulated as a tunneling problem. The following theorem is proved: for an electron confined to a quantum well of size W with an arbitrary conduction band energy profile $E_c(x)$ and maximum depth V_0, the bound state energies (E_1, E_2, E_3,…) can be found by adding a barrier of width d and height V_0 on either side of the quantum well and calculating the energies at which the transmission through the resulting resonant tunneling structure reaches unity. More precisely, the energies at which the transmission coefficient reaches unity converge towards the bound state energy levels when the thickness d tends to infinity. Numerically, the bound state energies can be determined with enough accuracy by using barrier thicknesses of a few nm.

1. Introduction

Simple bound state problems such as the particle-in-a-box, the attractive delta scatterer, the finite square well, and the harmonic oscillator and tunneling problems such as tunneling through a positive delta scatterer, a potential step, and a rectangular barrier are covered in most textbooks in quantum mechanics [1,2]. These problems have (sometimes lengthy) analytical solutions or can be reduced to the solutions of transcendental equations which can be solved numerically without too much effort [3,4]. A general approach to treat both bound state and tunneling problems based on the transfer matrix approach [5–11] has been used extensively in the past to study more complicated problems such as bound states of arbitrary quantum wells [12] and finite periodic potentials [13] and tunneling through finite repeated structures [14–17].

Hereafter, the power of the transfer matrix formalism [18] is used to show that the problem of finding the bound states of an arbitrary confined one-dimensional potential energy profile $E_c(x)$ can be reformulated as a tunneling problem. More specifically, the following theorem is proved: for an electron confined to a quantum well of size W with an arbitrary conduction band energy profile $E_c(x)$ and $E_c(x) = V_0$ for x outside the well, as shown in Fig. 1, the bound state energies ($E_1, E_2, E_3, \ldots$) can be found by adding two barriers of width d and height V_0 and calculating the energies at which the transmission probability $T(E)$ through the resonant tunneling structure so formed reaches unity. The energies at which the transmission coefficient reaches unity converge towards the bound state energy levels when the thickness d tends to infinity. The theorem is proved for the case of a spatially independent effective mass but can be easily extended to the case of a spatially varying effective mass.

Numerically, the bound state energies can be determined with enough accuracy by using barrier thicknesses of a few nm. The approach can easily implemented numerically and is illustrated hereafter with several numerical examples in which the conduction band energy profile within the quantum well is approximated by a series of randomly distributed steps where the conduction band profile is assumed to be constant.

The physics behind the connection between the bound state and tunneling problems is as follows: the transmission probability through the resonant tunneling device peaks whenever multiple reflections between the barriers lead to a build up of the probability density inside the well. This buildup corresponds to the formation of quasi-bound states in the well which are increasingly less leaky (i.e., their lifetime τ gets larger) as the width of the

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http://dx.doi.org/10.1016/j.physe.2014.07.020
1386-9477/

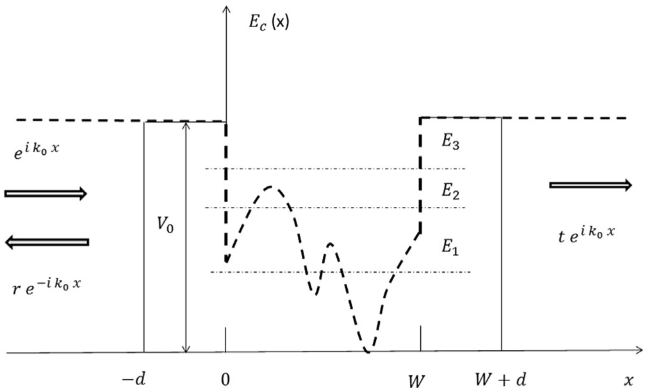

Fig. 1. Schematic of a quantum well (dashed line) of width W with an arbitrary potential energy profile and a maximum depth V_0. The zero of energy is selected as the minimum of $E_c(x)$ in the quantum well. The horizontal dash-dotted lines represent the three lowest bound state energies in the well, E_1, E_2, and E_3. The latter coincide with the energies of unit transmission for an electron incident from the left contact on a resonant tunneling device formed by adding cladding barriers of width d and height V_o when d is large; r and t are the reflection and transmission amplitudes, respectively, for an electron incident from the left with wavevector k_0.

barriers decreases. A quantitative estimate of the quasi-bound states lifetime can be obtained from the relation, $\Delta E\tau \sim \hbar$ where ΔE is the full width at half maximum of the resonant peaks in $T(E)$. As d increases ΔE decreases towards zero and τ gets larger, in agreement with an infinite lifetime for true bound states.

The paper is outlined as follows. Section 2 contains the description of the tunneling and bound states problems depicted in Fig. 1 in terms of the transfer matrix [18] and the connection between the two problems is established. Section 3 described several numerical examples to illustrate the theorem above. Section 4 contains our conclusions.

2. Proof of theorem

A. Tunneling problem: We first consider the tunneling through the resonant tunneling device shown in Fig. 1 using the bottom of the quantum well as the zero of energy. Calling V_o the maximum depth of the quantum well, the transfer matrix for each barrier on either side of the quantum well for $E \le V_0$ is given by [18]

$$W_B = \begin{pmatrix} csh(\kappa d) & \kappa sh(\kappa d) \\ \frac{sh(\kappa d)}{\kappa} & csh(\kappa d) \end{pmatrix} \tag{1}$$

where $\kappa = 1/\hbar\sqrt{2m(V_o - E)}$. For the resonant tunneling device, the overall transfer matrix is given by the product of the following three matrices [18]:

$$W_{TOT} = W_B W_{well} W_B, \tag{2}$$

where

$$W_{well} = \begin{pmatrix} \phi_1'(L) & \phi_2'(L) \\ \phi_1(L) & \phi_2(L) \end{pmatrix} \tag{3}$$

is the transfer matrix associated with the well region where the functions $\phi_1(x)$ and $\phi_2(x)$ are two linearly independent solutions of the Schröedinger equation satisfying the boundary conditions $\phi_1'(0) = 1$, $\phi_1(0) = 0$, $\phi_2'(0) = 0$, and $\phi_2(0) = 1$.

Performing the multiplication, we obtain

$$W_{TOT} = \cosh^2 \kappa d \begin{pmatrix} 1 & \kappa \tanh \kappa d \\ \frac{\tanh \kappa d}{\kappa} & 1 \end{pmatrix} \begin{pmatrix} \phi_1' + \frac{\phi_2'(L) \tanh \kappa d}{\kappa} & \kappa\phi_1'(L) \tanh \kappa d + \phi_2'(L) \\ \phi_1(L) + \frac{\phi_2(L) \tanh \kappa d}{\kappa} & \kappa\phi_1(L) \tanh \kappa d + \phi_2(L) \end{pmatrix}, \tag{4}$$

In the limit where $d \to \infty$, we have

$$W_{TOT} = csh^2 \kappa d \begin{pmatrix} 1 & \kappa \\ \frac{1}{\kappa} & 1 \end{pmatrix} \begin{pmatrix} \phi_1'(L) + \frac{\phi_2'(L)}{\kappa} & \kappa\phi_1'(L) + \phi_2'(L) \\ \phi_1(L) + \frac{\phi_2(L)}{\kappa} & \kappa\phi_1(L) + \phi_2(L) \end{pmatrix} \tag{5}$$

Multiply the last two matrices, we get for the elements of the matrix W_{TOT}

$$W_{TOT}^{11} = \cosh^2 \kappa d(\phi_1'(L) + \frac{\phi_2'(L)}{\kappa} + \kappa\phi_1(L) + \phi_2(L)), \tag{6}$$

$$W_{TOT}^{22} = W_{TOT}^{11}, \tag{7}$$

$$W_{TOT}^{12} = \cosh^2 \kappa d(\kappa\phi_1'(L) + \phi_2'(L) + \kappa^2\phi_1(L) + \kappa\phi_2(L)), \tag{8}$$

and

$$W_{TOT}^{21} = \cosh^2 \kappa d\left(\frac{\phi_1'(L)}{\kappa} + \frac{\phi_2'(L)}{\kappa} + \phi_1(L) + \frac{\phi_2(L)}{\kappa}\right). \tag{9}$$

The transmission probability through the resonant tunneling structure depends on the elements of the transfer matrix and reaches unity when the two following conditions are satisfied [16]

$$W_{12}^{TOT} = W_{21}^{TOT} = 0, \tag{10}$$

and

$$W_{11}^{TOT} + W_{22}^{TOT} = 2. \tag{11}$$

Using Eqs. (6)–(9), these last two conditions amount to the following requirement:

$$\kappa\phi_1'(L) + \phi_2'(L) + \kappa^2\phi_1(L) + \kappa\phi_2(L) = 0. \tag{12}$$

B. Bound state problem: Next we prove that Eq. (12) is also the condition equation which must be satisfied to find the bound states in the well. With the zero of energy at the bottom of the well, the solutions of the Schröedinger equation for the boundstate problem are given by

In region I ($x < 0$):

$$\psi_I = A_1 e^{\kappa x} + B_1 e^{-\kappa x}. \tag{13}$$

In region II ($0 < x < W$):

$$\psi_{II} = A_2\phi_1(x) + B_2\phi_2(x), \tag{14}$$

and in region III ($x > W$):

$$\psi_{III} = A_3 e^{\kappa(x-w)} + B_3 e^{-\kappa(x-w)}, \tag{15}$$

where $\kappa = 1/\hbar\sqrt{2m(V_0 - |E|)}$.

Matching the wavefunction and its derivative at $x=0$, we get the following relations between the coefficients (A_1, B_1) and $(A_2,\ B_2)$

$$\begin{pmatrix} \kappa & -\kappa \\ 1 & 1 \end{pmatrix} \begin{bmatrix} A_1 \\ B_1 \end{bmatrix} = \begin{pmatrix} \phi_1'(0) & \phi_2'(0) \\ \phi_1(0) & \phi_2(0) \end{pmatrix} \begin{bmatrix} A_2 \\ B_2 \end{bmatrix}. \tag{16}$$

Similarly at $x=W$, we get

$$\begin{pmatrix} \phi_1'(L) & \phi_2'(L) \\ \phi_1(L) & \phi_2(L) \end{pmatrix} \begin{bmatrix} A_2 \\ B_2 \end{bmatrix} = \begin{pmatrix} \kappa & -\kappa \\ 1 & 1 \end{pmatrix} \begin{bmatrix} A_3 \\ B_3 \end{bmatrix}. \tag{17}$$

The coefficient $B_1 = 0$ must be zero for the wavefunction to be well-behaved for $x < 0$.

Since $\phi_1'(0) = 1$, $\phi_1(0) = 0$, $\phi_2'(0) = 0$, and $\phi_2(0) = 1$, Eq. (16) becomes

$$A_2 = \kappa A_1, \tag{18}$$

and

$$B_2 = A_1. \tag{19}$$

Eq. (17) can be expanded as follows:

$$A_2\phi_1'(L) + B_2\phi_2'(L) = \kappa A_3 - \kappa B_3, \tag{20}$$