QUANTUM TUNNELING THROUGH A VERY NARROW TRIANGULAR POTENTIAL BARRIER EXACT AND WKB SOLUTION

Peter Ballo and Ladislav Harmatha

Slovak University of Technology, Ilkovičova 3, 812 19 Bratislava, Slovakia
E-mail: peter.ballo@stuba.sk

Received 30 April 2011; accepted 29 May 2011.

1. Introduction

The semiconductor industry has made amazing progress in last fifty years. The progress goes from big and robust elements to very tiny and efficient chips. Today the technology is on the way to cross all known technical as well as physical limits. Engineers are working with clusters of several atoms and currents of several electrons. This technology obviously needs quantum mechanical interpretation. Fortunately, today we have very good tool which has been created by collaborative work of many scientists in the past. Although today we have very complex and pretty theory its application without detailed knowledge is a dangerous matter. The motivation of this work is to show that manipulation with a very thin potential barrier needs not only a new kind of technology but also sensible application of numerical techniques. The goal of this paper is to advertise on difference between exact and WKB solutions if are applied on 1 nm thin potential barrier.

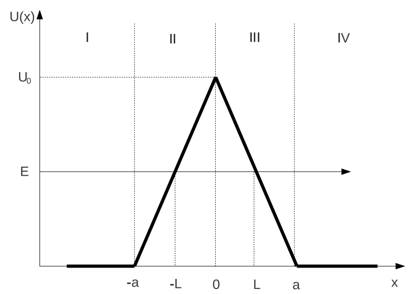

Fig.1: *The triangular barrier shape which is used in simulation. The shape provides a good approximation for real thin slide semiconductor structures. The thickness is 2a=1nm and the barrier height is U0=3eV. Energy E means instant energy of interaction between quantum mechanical particle and potential barrier.*

2. Theory

The barrier is assumed as a triangular shape with constant increase and decrease potential from left to right as is shown in Fig.1. As usual [1] the space is divided into four subspaces. The subspaces are referred as I. – IV. From mathematical point of view the property of subspaces are described in Eqs. 1.

$$\begin{array}{ll} U(x)=0 & x<-a \\ U(x)=U_0(1+x/a) & -a\le x<0 \\ U(x)=U_0(1-x/a) & 0\le x<a \\ U(x)=0 & x\ge a \end{array} \tag{1}$$

To simplify further calculations we introduce two new variables k_0 and q_0:

$$k_0^2 = 2mE/\hbar^2 \qquad q_0^2 = 2mU_0/\hbar^2 \tag{2}$$

Solution of Schrödinger equation depends on actual subspace. In two subspaces (I. and IV.) the particle is free. In other two subspaces (II. and III.) the particle is accelerated and decelerated, respectively. The solution can be written as a superposition of left and right moving waves which obey:

$$\begin{array}{ll} \Psi(x)=e^{ik_0x}+\alpha e^{-ik_0x} & x<-a \\ \Psi(x)=\beta Ai(\zeta)+\gamma Bi(\zeta) & -a\le x<0 \\ \Psi(x)=\delta Ai(\eta)+\varepsilon Bi(\eta) & 0\le x<a \\ \Psi(x)=\vartheta e^{ik_0x} & x\ge a \end{array} \tag{3}$$

ζ and η are transformed variables containing information about the potential barrier [1]. The coefficients $\alpha,\beta,\gamma,\delta,\varepsilon$ and ϑ have to be found from the boundary conditions of the wave function at x = -a, x = 0 and x = a. The wave function and its derivative have to be continuous everywhere, so we have got (after some algebra) six equations:

$$\begin{array}{l} e^{-ik_0a}+\alpha e^{ik_0a}=\beta Ai(-\rho)+\gamma Bi(-\rho) \\ i\sqrt{\rho}(e^{-k_0a}-\alpha e^{ik_0a}=\beta Ai'(-\rho)+\gamma Bi'(-\rho) \\ \beta Ai(\mu)+\gamma Bi(\mu)=\delta Ai(\mu)+\varepsilon Bi(\mu) \\ \beta Ai'(\mu)+\gamma Bi'(\mu)=-\delta Ai'(\mu)-\varepsilon Bi'(\mu) \\ \delta Ai(-\rho)+\varepsilon Bi(-\rho)=\vartheta e^{ik_0a} \\ \delta Ai'(-\rho)+\varepsilon Bi'(-\rho)=-i\sqrt{\rho}\vartheta e^{ik_0a} \end{array} \tag{4}$$

where ρ and μ are new variables expressed as:

$$\begin{array}{l} \rho\equiv k_0^2a^{\frac{2}{3}}q_0^{-\frac{4}{3}}=(q_0a)^{\frac{2}{3}})(k_0/q_0)^2 \\ \mu\equiv a^{\frac{2}{3}}q_0^{-\frac{4}{3}}(q_0^2-k_0^2)=(q_0a)^{\frac{2}{3}}(1-k_0^2/q_0^2) \end{array} \tag{5}$$

After other portion of algebra we have got expression for transmission coefficient T:

$$T\equiv|\vartheta|^2=\frac{\rho}{\{[Bi(\mu)Ai'(-\rho)-Ai(\mu)Bi(-\rho)]^2+\rho[Bi(\mu)Ai(-\rho)-Ai(\mu)Bi(-\rho)]^2\}} \times\frac{1}{\{[Bi'(\mu)Ai'(-\rho)-Ai'(\mu)Bi(-\rho)]^2+\rho[Bi'(\mu)Ai(-\rho)-Ai'(\mu)Bi(-\rho)]^2\}} \tag{6}$$

where *Ai(x)* and *Bi(x)* are Airy functions. Both are solutions of Airy equation:

$$f''(x) - kf(x) = 0 \tag{7}$$

and *Ai'(x)* and *Bi'(x)* are derivatives of Airy functions. The solution (6) is exact in the frame of quantum mechanical theory. The key stone of quasi-classical approximation is the fact that the wave changes in wavelength

$$\lambda(x) = \frac{\hbar}{\sqrt{2m[E - U(x)]}} \tag{8}$$

must be small over one wavelength. This could be expressed as:

$$\lambda(x) = \frac{1}{k_0} \rightarrow \frac{d\lambda(x)}{dx} = 0 \tag{9}$$

Last expression is rewritten using ρ and μ:

$$\lambda(x) = (\frac{a}{q_0^2})^{\frac{1}{3}} \frac{1}{i\sqrt{\rho}} \rightarrow \frac{d\lambda}{dx} \equiv \frac{d\lambda}{d\rho}\frac{d\rho}{dx} = -\frac{1}{2i\rho^{\frac{3}{2}}}$$

$$\lambda(x) = (\frac{a}{q_0^2})^{\frac{1}{3}} \frac{1}{i\sqrt{\mu}} \rightarrow \frac{d\lambda}{dx} \equiv \frac{d\lambda}{d\mu}\frac{d\mu}{dx} = -\frac{1}{2i\mu^{\frac{3}{2}}} \tag{10}$$

If the condition of quasi-classical solution $|d\lambda / dx| \quad <<< 1$ (WKB approximation) is applied we could write:

$$|\rho| >>> 1 \text{ and } |\mu| >>> 1 \tag{11}$$

Using asymptotic expressions of Airy functions for t>>>1:

$$\begin{aligned}
&Ai(t) \approx t^{-\frac{1}{4}} e^{x} \quad Ai'(t) \approx t^{\frac{1}{4}} e^{x} \\
&Bi(t) \approx \frac{1}{2} t^{-\frac{1}{4}} e^{-x} \quad Bi'(t) \approx -\frac{1}{2} t^{-\frac{1}{4}} e^{-x} \\
&Ai(-t) \approx t^{-\frac{1}{4}} cos(x + \frac{\pi}{4}) \quad Ai'(-t) \approx t^{\frac{1}{4}} sin(x + \frac{\pi}{4}) \\
&Bi(-t) \approx t^{-\frac{1}{4}} sin(x + \frac{\pi}{4}) \quad Bi'(-t) \approx -t^{\frac{1}{4}} cos(x + \frac{\pi}{4})
\end{aligned} \tag{12}$$

After some algebra and application of asymptotic expressions (12) the expression (6) could be rewritten in more simple form:

$$T \approx e^{-\frac{8}{3}\mu^{\frac{3}{2}}} = e^{-\frac{8}{3}\frac{a\sqrt{2m}}{\hbar U_0}(U_0 - E)^{\frac{3}{2}}} \tag{13}$$

And in more usual form: $T \approx e^{-2\int_{-L}^{L}\sqrt{\frac{2m}{\hbar^2}|U(x)-E|}dx}$ (14)

Equation (14) gives transmission coefficient in WKB approximation. The equation could be applied on general form of potential barrier if the condition (9) is applicable. This is obviously not true in the case of abrupt junction with potential rapid slope. In Fig. 2 is plotted transparency T of a triangle potential barrier which is schematically plotted in Fig. 1. Abscissa axis shows energy E in ratio scale of barrier amplitude U_0. Ordinate axis gives potential barrier transparency T. Relation between exact and WKB approximation shows that the error could be more as 100 percent if the thickness of potential barrier is about 1nm.

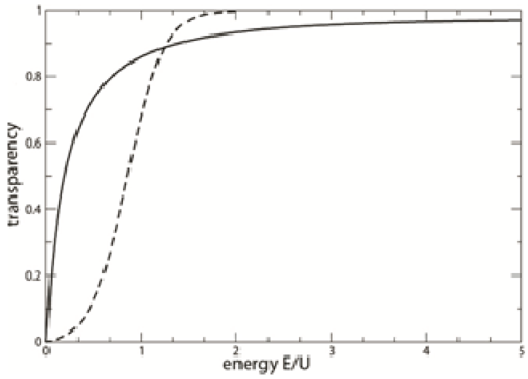

Fig 2: *Transparency T of a triangle potential barrier which is schematically plotted in Fig. 1. Abscissa axis shows energy E in ratio scale of barrier amplitude U0. Ordinate scale gives potential barrier transparency T. Exact solution according Equation (6) is plotted in the solid line. WKB approximation is plotted in the dashed line.*

3. Conclusion

We have investigated the quantum-mechanical transmission of an electron in narrow potential barrier. It has been shown that application of WKB approximation could give enormous error if the slope of potential is rapid. Edification of this work is that unreasonable application of numerical approximations without the deep knowledge of theory should give wrong result. This we should remember every second, every day.

Acknowledgment

This publication is the result of the project implementation: CENTE II, ITMS code 26240120019, supported by the Research & Development Operational Program funded by the ERDF and by grant VEGA 1/0507/09 of the Ministry of Education of the Slovak Republic.

References

[1] V. I. Kogan, V. M. Galickij: Sbornik zadač po kvantovoj mechanike, Goštechizdat, Moskva (1956).