

# อภินันทนาการ



สำนักหอสมุด



รายงานวิจัยฉบับสมบูรณ์

โครงการ การใช้การประมาณ WKB สำหรับบ่อพลังงานศักย์ที่มีการเปลี่ยนแปลง  
อย่างฉับพลัน

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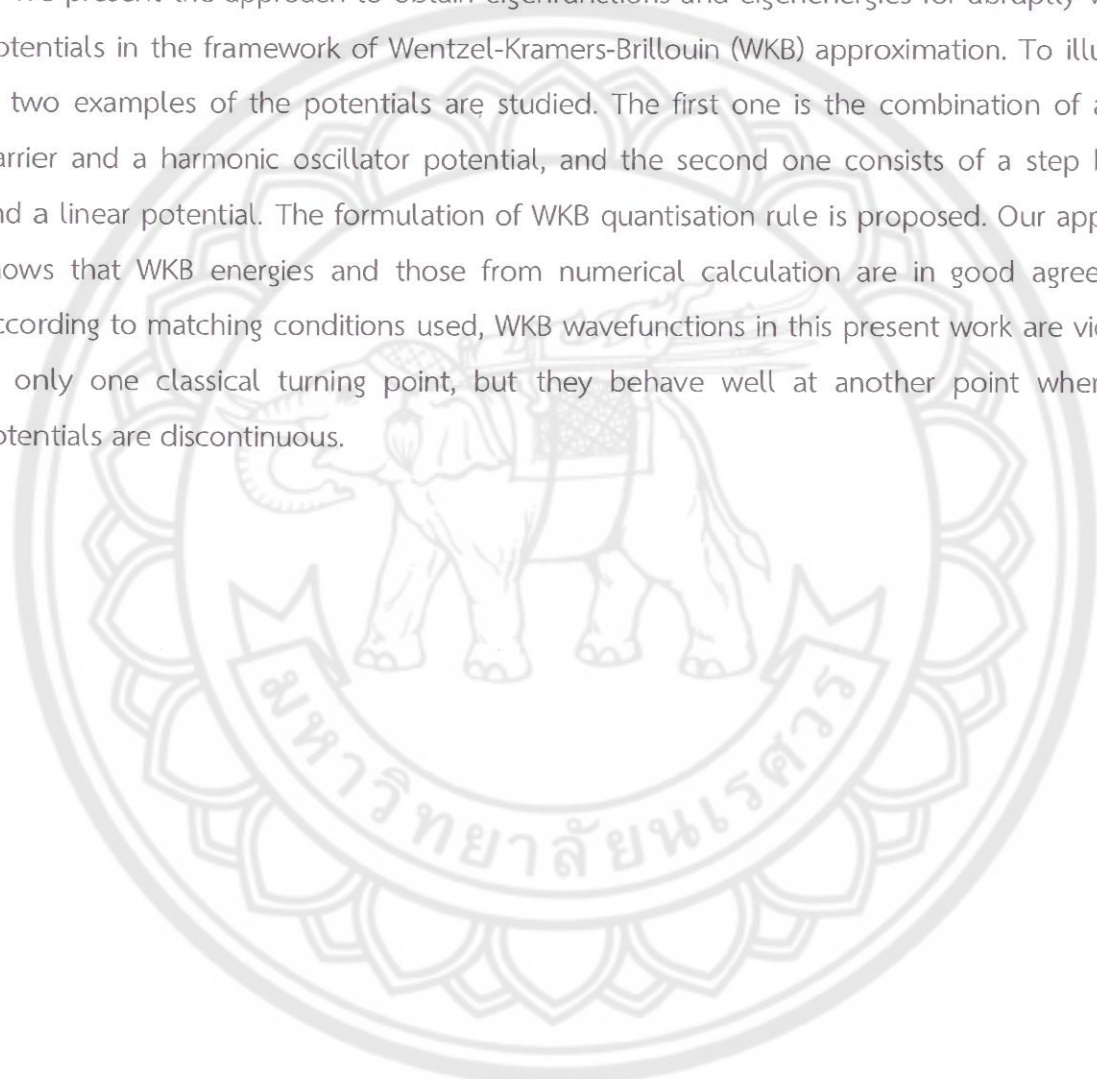
## บทคัดย่อ

โครงการนี้เกี่ยวข้องกับการคำนวณฟังก์ชันคลื่นและพลังงานของอนุภาคที่ถูกกักขังในบ่อพลังงานศักย์ที่มีการเปลี่ยนแปลงอย่างรวดเร็วโดยวิธีการประมาณ WKB เพื่อให้เห็นการนำไปใช้อย่างชัดเจนเราได้นำเสนอวิธีนี้กับบ่อพลังงาน 2 แบบ แบบแรกเป็นการผสมกันของฟังก์ชันขั้นบันไดและพลังงานศักย์แบบฮาร์มอนิก แบบที่สองเป็นการผสมกันของฟังก์ชันขั้นบันไดและพลังงานศักย์แบบเชิงเส้น สูตรการคำนวณพลังงานของอนุภาคโดยใช้กฎของ WKB ได้ถูกพัฒนาขึ้นในงานนี้ ซึ่งผลจากการคำนวณโดยวิธี WKB สอดคล้องกับผลจากการคำนวณโดยวิธีเชิงตัวเลขอย่างสูงแต่การคำนวณโดยวิธีเชิงตัวเลขนั้นใช้เวลามากกว่ามาก อย่างไรก็ตามเราพบว่า ฟังก์ชันคลื่นของอนุภาคจากวิธี WKB มีพฤติกรรมไม่เหมาะสมที่จุดวกกลับหนึ่งจุด และมีพฤติกรรมที่เหมาะสมอีกหนึ่งจุดที่ตำแหน่งซึ่งพลังงานศักย์ไม่ต่อเนื่อง



## Abstract

We present the approach to obtain eigenfunctions and eigenenergies for abruptly varying potentials in the framework of Wentzel-Kramers-Brillouin (WKB) approximation. To illustrate it, two examples of the potentials are studied. The first one is the combination of a step barrier and a harmonic oscillator potential, and the second one consists of a step barrier and a linear potential. The formulation of WKB quantisation rule is proposed. Our approach shows that WKB energies and those from numerical calculation are in good agreement. According to matching conditions used, WKB wavefunctions in this present work are violated at only one classical turning point, but they behave well at another point where the potentials are discontinuous.





## Executive Summary

โครงการนี้ได้เสนอวิธีการใช้ WKB สำหรับบ่อพลังงานศักย์ที่มีการเปลี่ยนแปลงอย่างฉับพลันซึ่งประกอบด้วยกำแพงศักย์ที่ตั้งฉากที่จุดวงกลับซึ่งพลังงานศักย์เปลี่ยนแปลงช้า ฟังก์ชันคลื่นจากวิธี WKB มีพฤติกรรมไม่เหมาะสมเพราะการหายไปของโมเมนต์ในทางตรงกันข้ามอีกจุดวงกลับหนึ่งซึ่งพลังงานศักย์ยกขึ้นอย่างรวดเร็ว ฟังก์ชันคลื่นจากวิธี WKB แสดงพฤติกรรมที่เหมาะสมและคล้ายกับผลจากการคำนวณเชิงตัวเลข เราจึงสามารถเชื่อมฟังก์ชันคลื่นนี้ได้ที่จุดวงกลับนี้ พลังงานที่ได้จากวิธี WKB มีความสอดคล้องกับผลจากการคำนวณเชิงตัวเลขโดยเฉพาะสถานะที่มีพลังงานสูงๆ แม้ว่าการกระจายตัวของ ฟังก์ชันคลื่นจากวิธี WKB จะ ผิดพลาดที่จุดวงกลับซึ่งพลังงานศักย์เปลี่ยนแปลงอย่างช้าๆแต่การกระจายตัวดังกล่าวก็มีความสอดคล้องกับผลจากการคำนวณเชิงตัวเลขในบริเวณที่เหลือเป็นอย่างดี

วิธี WKB ที่พัฒนาขึ้นนี้มีประโยชน์อย่างมาก มันสามารถนำไปประยุกต์ใช้กับพลังงานศักย์ที่ประกอบด้วยกำแพงศักย์ตั้งฉากเช่นพลังงานศักย์แบบสามเหลี่ยมซึ่งพบได้มากที่รอยต่อระหว่างแผ่นสารกึ่งตัวนำสองชนิด ในกรณีของรอยต่อระหว่างสองสารกึ่งตัวนำที่มีความต่างของแถบพลังงานมากๆ วิธี WKB อาจไม่จำเป็นเนื่องจากสามารถประมาณพลังงานศักย์ได้เป็นพลังงานศักย์แบบสามเหลี่ยมที่มีด้านหนึ่งเป็นอนันต์ได้ แต่หากความแตกต่างของแถบพลังงานไม่มากพอ ฟังก์ชันคลื่นจะสามารถทะลุทะลวงเข้าไปในพลังงานศักย์ได้ ทำให้ วิธี WKB ที่พัฒนาขึ้นในงานนี้มีความจำเป็นทันที นอกจากนี้วิธี WKB นี้ยังสามารถนำไปใช้กับสมการชโรดิงเงอร์ในหลายมิติได้อีกเหมือนกับวิธี WKB ทั่วไป แต่ต้องมีการปรับเปลี่ยนปัญหาในหลายมิติให้กลายเป็นปัญหาในหนึ่งมิติเสียก่อน

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## 1. บทนำ

วิธี WKB เป็นวิธีการประมาณผลเฉลยของสมการชโรดิงเงอร์ ซึ่งสามารถนำไปประยุกต์ใช้แก้สมการอนุพันธ์ในฟิสิกส์สาขาต่างๆ [1-4] สำหรับกลศาสตร์ควอนตัมมันถูกเข้าใจว่าสามารถนำไปใช้ได้กับพลังงานศักย์ที่มีการเปลี่ยนแปลงอย่างช้าๆ เท่านั้นเมื่อเทียบกับความยาวคลื่นของฟังก์ชันคลื่น การประมาณนี้นำไปสู่การสั้นของฟังก์ชันคลื่นในรูปแบบ [5]

$$\Psi(x) = \frac{1}{\sqrt{p(x)}} \exp \left[ \pm \frac{i}{\hbar} \int p(x) dx \right] \quad (1)$$

ในบริเวณที่กลศาสตร์แบบฉบับอนุญาต ( $E > V$ ) และการลดลงของฟังก์ชันคลื่นในรูปแบบ

$$\Psi(x) = \frac{1}{\sqrt{|p(x)|}} \exp \left[ \pm \frac{1}{\hbar} \int |p(x)| dx \right] \quad (2)$$

ในบริเวณที่กลศาสตร์แบบฉบับไม่อนุญาต ( $E < V$ ) เมื่อ  $p(x)$  เป็นโมเมนตัมของอนุภาคที่มีพลังงาน  $E$  ที่บริเวณใกล้จุดวกกลับ ฟังก์ชันคลื่นจากวิธี WKB มีพฤติกรรมไม่เหมาะสมเนื่องจากตัวส่วนในสมการที่ (1) และ (2) มีค่าเข้าสู่นันต์ [6] ผลก็คือฟังก์ชันคลื่นไม่สามารถเชื่อมด้วยวิธีธรรมดา

เพื่อให้ได้ พลังงานของอนุภาคที่ถูกกักขัง ฟังก์ชันคลื่นในสมการที่ (1) และ (2) จะถูกเชื่อมโดยสูตรการเชื่อมเฉพาะ [7] ซึ่งพิสูจน์จากการทำให้พลังงานศักย์มีความเป็นเชิงเส้นที่จุดวกกลับ แล้วได้พลังงานจากวิธี WKB ว่า

$$\int_{x_1}^{x_2} \sqrt{2m[E_n - V(x)]} dx = \frac{h}{2} \left( n - \frac{1}{2} \right), \quad (3)$$

เมื่อ  $x_1$  และ  $x_2$  คือจุดวกกลับ

วิธีนี้สามารถนำไปประยุกต์ใช้กับพลังงานศักย์ที่มีการเปลี่ยนแปลงอย่างฉับพลันโดยเฉพาะกับพลังงานศักย์ที่มีกำแพงศักย์อนันต์ [5,8,9] ในกรณีนี้พลังงานหาได้โดยใช้เงื่อนไขขอบเขตซึ่งฟังก์ชันคลื่นหายไปขอบกำแพงศักย์อนันต์ ตัวอย่างการใช้พลังงานศักย์เหล่านี้ เช่น กำแพงศักย์อนันต์ขนานสองข้างและกำแพงศักย์อนันต์ขนานด้วยพลังงานศักย์แบบฮาร์โมนิกซึ่ง วิธี WKB ให้ค่าที่ถูกต้องเท่าผลเฉลยแน่นอนตรง [5,9]



อย่างไรก็ตามพลังงานศักย์ไม่ได้เป็นดังเช่นกรณีดังกล่าวเสมอไป บางครั้งมันมีค่าสูงขึ้นอย่างทันทีทันใด แล้วจบที่ค่าคงที่หนึ่งๆเช่น พลังงานศักย์สี่เหลี่ยมจากสารกึ่งตัวนำที่มีช่องว่างพลังงานแคบขนานข้างด้วยสารกึ่งตัวนำที่มีช่องว่างพลังงานกว้าง มันดูเหมือนว่าสูตรการเชื่อมไม่สามารถนำมาใช้ได้ในกรณีนี้เพราะพลังงานศักย์ไม่สามารถประมาณด้วยกราฟเชิงเส้นได้ที่จุดวกกลับ เท่าที่เราทราบไม่เคยมีใครใช้วิธี WKB กับพลังงานศักย์เหล่านี้นมาก่อน

ในงานนี้เราเสนอวิธีการใช้การประมาณ WKB เพื่อหาผลเฉลยของสมการชโรดิงเงอร์ที่มีพลังงานศักย์ซึ่งเปลี่ยนแปลงอย่างรวดเร็ว เพื่อให้เข้าใจวิธีใช้อย่างชัดเจน เราใช้วิธีนี้กับตัวอย่างสองตัวอย่างได้แก่ พลังงานศักย์แบบฮามอนิกที่ถูกปรับปรุง และพลังงานศักย์แบบสามเหลี่ยมที่กำลังแ่งศักย์คงที่ซึ่งใช้กันอย่างแพร่หลายในฟิสิกส์สาขาสารกึ่งตัวนำโดยพลังงานศักย์นี้เป็นต้นแบบของพลังงานศักย์สารกึ่งตัวนำสองตัวที่มีช่องว่างพลังงานต่างกัน เช่น พลังงานศักย์ที่บริเวณรอยต่อของ GaAs-AlGaAs ที่ซึ่ง GaAs และ AlGaAs แทนด้วยกำลังแ่งศักย์เชิงเส้นและกำลังแ่งศักย์ขึ้นบันไดตามลำดับเพื่อให้เห็นถึงความแม่นยำของวิธี WKB ที่พัฒนาเราได้เปรียบเทียบพลังงานและฟังก์ชันคลื่นกับการคำนวณเชิงเส้นซึ่งสามารถใช้ได้กับพลังงานศักย์ทุกรูปแบบอยู่แล้วแต่ใช้เวลาในการคำนวณนานกว่ามาก แม้ว่าการคำนวณเชิงเส้นจะใช้ผลเฉลยที่มีความแม่นยำสูง คำตอบที่ได้เป็นเพียงชุดของจุดซึ่งไม่ได้ให้ความเข้าใจใดๆ กับผู้ใช้เลยแต่วิธี WKB สามารถให้ผลเฉลยที่วิเคราะห์ได้ อย่างน้อยผู้ใช้ก็สามารถเข้าใจการสั่นและการลดลงของฟังก์ชันคลื่น และยังสามารถวิเคราะห์ระดับพลังงานที่เป็นไปได้อีกด้วย

## 2. การวิเคราะห์วิธี WKB สำหรับบ่อพลังงานศักย์ที่เปลี่ยนแปลงอย่างรวดเร็ว

We begin this section with the one-dimensional Schrödinger equation:

$$\left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \Psi(x) = E\Psi(x), \quad (4)$$

where  $V(x)$  is a confined potential which rises suddenly at  $x = 0$ . The general model of our considered potential is given by

$$V(x) = \begin{cases} V_1(x) & x < 0 \\ V_2(x) & x \geq 0. \end{cases} \quad (5)$$

$V_1(x)$  and  $V_2(x)$  are arbitrary functions which are not connected each other at  $x = 0$ . In our model, the vertically finite wall is on the side of  $V_1$ , leading to a turning point localised at  $x_1 = 0$  and another one at  $x_2$  as depicted in Fig. 1. We then express the quantities in the following units:  $x = \tilde{x}a$ ,  $E = \tilde{E}E_0$ , and  $V = \tilde{V}E_0$ , where  $E_0 = \hbar^2/(ma^2)$  and  $a$  is an arbitrary fixed length. Now, the Schrödinger equation (4) becomes

$$\left[ -\frac{1}{2} \frac{\partial^2}{\partial \tilde{x}^2} + \tilde{V}(\tilde{x}) \right] \Psi(\tilde{x}) = \tilde{E}\Psi(\tilde{x}), \quad (6)$$

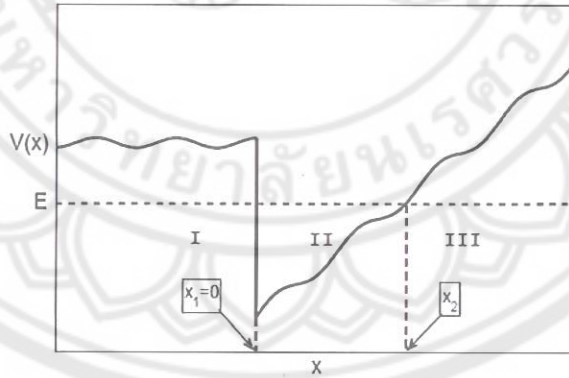


FIG. 1. An attractive potential  $V(x)$  varying abruptly at  $x = 0$ . For a particle with energy  $E$ , the symbols I and III represent the classically forbidden regions, while II represents the classically allowed region.



Note that the tilde will be dropped in the following expression for convenience. It is not a good idea to apply the conventional energy quantisation in equation (3) to our considered potential because of two reasons. Firstly, equation (3) is derived from the assumption that a potential  $V(x)$  depends linearly on the variable  $x$  at the turning points. This assumption is obviously violated at  $x = 0$ . Secondly, integrating from  $x_1$  to  $x_2$  in equation (3) suggests that the approximated eigenenergies are totally independent of the potential in the classically forbidden regions. This is a bad approximation for the investigated potential since  $V_1(x)$ , the potential in region I, indicates how far quantum wavefunctions penetrate into the nonclassical region, and certainly influences the eigenenergies. In other words, it is unreasonable that varying the potential  $V_1(x)$  results in unchanged energies.

We propose that the WKB theory can still be used. The decaying WKB wavefunctions corresponding to the dimensionless Schrödinger equation (6) in the first and the third regions in Fig. 1 are

$$\Psi_I(x) = \frac{A}{\sqrt{\kappa}} \exp \left[ - \int_x^{x_1} \kappa(x') dx' \right] \quad (7)$$

and

$$\Psi_{III}(x) = \frac{B}{\sqrt{\kappa}} \exp \left[ - \int_{x_2}^x \kappa(x') dx' \right], \quad (8)$$

respectively, where  $A$  and  $B$  are the normalising constants and  $\kappa(x) = \sqrt{2(V - E)}$ . Note that the subscripts refer to the regions where the wavefunctions exist. If  $V_2(x)$  does not change abruptly, we can use the connection formulae to connect the decaying wavefunctions  $\Psi_{III}$  to the oscillating wavefunctions in region II, obtaining

$$\Psi_{II}(x) = \frac{2B}{\sqrt{k}} \sin \left[ \int_x^{x_2} k(x') dx' + \frac{\pi}{4} \right], \quad (9)$$

where  $k(x) = \sqrt{2(E - V)}$ . As discussed before, one should not join the wavefunction  $\Psi_I$  and wavefunction  $\Psi_{II}$  together at  $x = 0$  by using the connection formulae. However, we notice that the WKB wavefunctions in both regions behave well around the turning point  $x = 0$ ; therefore, the wavefunctions can be matched normally by the boundary condition:

$$\left. \frac{\Psi'_I}{\Psi_I} \right|_{x=0} = \left. \frac{\Psi'_{II}}{\Psi_{II}} \right|_{x=0}. \quad (10)$$

Now, the coefficients  $A$  and  $B$  are disappeared, and the quantised energies are expected to be obtained after imposing the condition. To demonstrate the advantage of this WKB analysis, we will calculate the eigenenergies and eigenstates associated with the considered potential in the following two examples.

## 2.1 ป่อพลังงานศักย์ของฟังก์ชันขั้นบันไดและฮาร์มอนิก

The step-harmonic potential which contains a vertically finite wall is of the form discussed in equation (5). It is formed by the step function  $V_0\Theta(-x)$  and the harmonic oscillator potential  $Kx^2\Theta(x)$ , where  $\Theta(x)$  is the Heaviside step function and  $K$  is a constant indicating the width of the quantum well. To get the Schrödinger equation in the dimensionless form of equation (6), we measure energies in the unit of  $E_0 = \hbar^2/(ma^2)$ , where  $a$  is the length  $[\hbar^2/(2Km)]^{1/4}$ . The potential is consequently expressed as

$$V(x) = \begin{cases} V_0 & x < 0 \\ x^2/2 & x \geq 0, \end{cases} \quad (11)$$

as depicted in Fig 2. Before constructing WKB wavefunctions, we need to calculate the

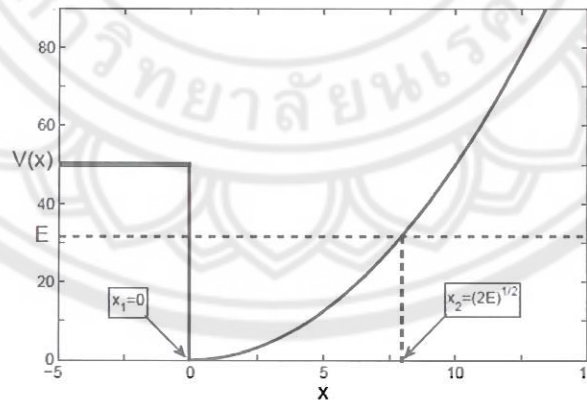


FIG. 2. The step-harmonic potential with the classical turning points at  $x_1 = 0$  and  $x_2 = \sqrt{2E}$ . The potential  $V(x)$  and distance  $x$  are in units of  $E_0 = \hbar\sqrt{\frac{2K}{m}}$  and  $a = \left(\frac{\hbar^2}{2Km}\right)^{1/4}$  respectively.

and

$$\begin{aligned}\int_x^{x_2} k(x') dx' &= \int_x^{\sqrt{2E}} \sqrt{2 \left( E - \frac{x'^2}{2} \right)} dx' \\ &= \frac{E\pi}{2} - \left[ \frac{x}{2} \sqrt{2E - x^2} + E \tan^{-1} \left( \frac{x}{\sqrt{2E - x^2}} \right) \right].\end{aligned}\quad (13)$$

In the above calculation, the classical turning points are localised at  $x_1 = 0$  and  $x_2 = \sqrt{2E}$ . We straightforwardly substitute equations (12) and (13) into the WKB wavefunctions  $\Psi_I$  (7) and  $\Psi_{II}$  (9), then applying the boundary condition (10) to get the energy quantisation rule:

$$\sqrt{V_0 - E} = -\sqrt{E} \cot \theta, \quad (14)$$

where  $\theta = \left( \frac{E\pi}{2} + \frac{\pi}{4} \right)$ .

Our WKB energies are compared with ones from the finite difference method which are converged and accurate to 5 decimal places. Table I shows that WKB energies and those due to the numerical calculation are in very good agreement; the percentage error is less than 0.5 for all trial values of  $V_0$ . We notice that the approximated values are always greater than the numerical ones. The number of confined states is determined by the strength of the potential  $V_0$ ; it increases as the potential is stronger. For a given value of  $V_0$ , the agreement between two independent methods is improved with increasing  $n$ . That is, the approximation is better for higher energy states. This is the conventional trend in the WKB method, which can be explained by the inspirational assumption that a potential  $V(x)$  changes slowly compared with wavelengths of quantum wavefunctions. In other words, the distance on which a potential changes significantly is large compared with quantum wavelengths. Therefore, high-energy excited states with small wavelengths seem to satisfy the assumption more than the low-lying confined states. For each value of  $n$ , the table shows WKB approximation gives higher accurate results when the potential  $V_0$  is stronger. When the potential  $V_0$  becomes an infinity well, a quantum wavefunction cannot tunnel through the side. In this case, we have the boundary condition

$$\Psi_{II}(x = 0) = 0, \quad (15)$$



resulting in the quantised energies

$$E = n - \frac{1}{2} \quad \text{for } n = 2, 4, 6, \dots \quad (16)$$

This is the exact solution of the half-space harmonic oscillator which confirms that WKB calculation is a good approximation for high strength of the barrier  $V_0$ .

After obtaining eigenenergies, we use them to calculate WKB eigenfunctions in those three regions and combine them together to get total WKB wavefunctions ( $\Psi^{\text{WKB}} = \Psi_{\text{I}} + \Psi_{\text{II}} + \Psi_{\text{III}}$ ). The first 4 eigenstates corresponding to the step-harmonic potential with  $V_0 = 50$  are shown in Fig 3. We find WKB eigenstates have the same behaviour as those from the finite difference method everywhere except the region around the turning point  $x_2$ . They go to infinity at the turning point, but behave very well at another point  $x_1 = 0$ . The local momentum  $p(x)$  plays a key role in the distribution of WKB wavefunctions at the turning points. At  $x_2$  the energies of trapped states are equal to the potential, resulting in  $p(x_2) = 0$  and inappropriate distribution of WKB wavefunctions; on the other hand, at  $x_1$  the quantised energies that are always less than  $V_0$  lead to  $p(x_1) \neq 0$  and appropriate distribution of the wavefunctions.

	$V_0=10$				$V_0=50$		
	E(numerical)	E(WKB)	Percentage error		E(numerical)	E(WKB)	Percentage error
$n=1$	1.26217	1.26820	0.47762	$n=1$	1.39055	1.39323	0.19261
$n=2$	3.12085	3.12253	0.05376	$n=2$	3.33290	3.33373	0.02495
$n=3$	4.99927	5.00000	0.01467	$n=3$	5.28869	5.28911	0.00799
$n=4$	6.87711	6.87747	0.00529	$n=4$	7.25102	7.25128	0.00364
	$V_0=90$				$V_0=130$		
	E(numerical)	E(WKB)	Percentage error		E(numerical)	E(WKB)	Percentage error
$n=1$	1.41785	1.41983	0.13978	$n=1$	1.43139	1.43304	0.11470
$n=2$	3.37530	3.37592	0.01845	$n=2$	3.39612	3.39664	0.01527
$n=3$	5.34298	5.34330	0.00600	$n=3$	5.36944	5.36971	0.00500
$n=4$	7.31574	7.31594	0.00278	$n=4$	7.34702	7.34719	0.00234

TABLE I. Comparison between numerical and WKB energies for various values of the barrier  $V_0$  and for several low-lying states. All eigenenergies and potentials are measured in the unit of  $E_0 = \hbar\sqrt{\frac{2K}{m}}$ .

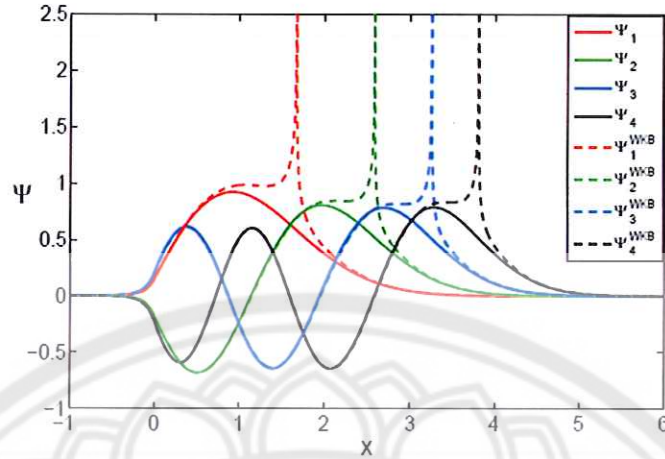


FIG. 3. Comparison between the numerical wavefunctions  $\Psi_n$  and WKB wavefunctions  $\Psi_n^{\text{WKB}}$  corresponding to the step-harmonic potential with  $V_0 = 50$  for several values of quantum number  $n$ . The distance  $x$  is in the unit of  $a = \left(\frac{\hbar^2}{2Km}\right)^{1/4}$ .

## 2.2 ป็อพลังงานศักย์ของฟังก์ชันขั้นบันไดและเชิงเส้น

The next example we will show is a particle in the step-linear potential. It is the potential with a vertical wall at  $x = 0$ , containing the step function  $V_0\Theta(-x)$  and the linear potential  $Kx\Theta(x)$ , where  $K$  is a constant determining the slope of the linear term. The Schrödinger equation can be written in the dimensionless form of equation (6) by introducing the energy unit  $E_0 = \hbar^2/(ma^2)$ , where  $a = [\hbar^2/(2Km)]^{1/3}$ . Now, the dimensionless potential becomes

$$V(x) = \begin{cases} V_0 & x < 0 \\ x/2 & x \geq 0, \end{cases} \quad (17)$$

where the classical turning points are at  $x_1 = 0$  and  $x_2 = 2E$ , shown in Fig 4. Again, we start finding WKB wavefunctions by calculating the integral

$$\begin{aligned} \int_x^{x_2} k(x')dx' &= \int_x^{2E} \sqrt{2\left(E - \frac{x'}{2}\right)}dx' \\ &= \frac{2}{3}(2E - x)^{3/2}. \end{aligned} \quad (18)$$



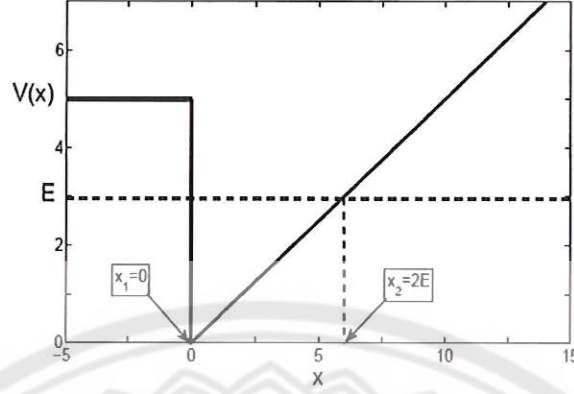


FIG. 4. The step-linear potential with the classical turning points at  $x_1 = 0$  and  $x_2 = 2E$ . The potential  $V(x)$  and distance  $x$  are in units of  $E_0 = [(2\hbar K)^2/m]^{1/3}$  and  $a = [\hbar^2/(2Km)]^{1/3}$  respectively.

Substitute equations (12) and (18) into the WKB wavefunctions  $\Psi_I$  (7) and  $\Psi_{II}$  (9), and impose the boundary condition (10) to obtain the energy quantisation rule:

$$E(V_0 - E)^{1/2} = \frac{\sqrt{2}}{16} - E^{3/2} \cot(\theta), \quad (19)$$

where  $\theta = \frac{4\sqrt{2}}{3} E^{3/2} + \frac{\pi}{4}$ .

	$V_0=10$				$V_0=50$		
	E(numerical)	E(WKB)	Percentage error		E(numerical)	E(WKB)	Percentage error
$n=1$	1.05529	1.04625	0.85661	$n=1$	1.11887	1.10993	0.79877
$n=2$	1.92834	1.92524	0.16090	$n=2$	1.99364	1.99057	0.15410
$n=3$	2.64297	2.64126	0.06489	$n=3$	2.70982	2.70812	0.06268
$n=4$	3.27445	3.27331	0.03472	$n=4$	3.34278	3.34166	0.03369
	$V_0=90$				$V_0=130$		
	E(numerical)	E(WKB)	Percentage error		E(numerical)	E(WKB)	Percentage error
$n=1$	1.13171	1.12278	0.78924	$n=1$	1.13800	1.12907	0.78474
$n=2$	2.00657	2.00350	0.15302	$n=2$	2.01289	2.00982	0.15252
$n=3$	2.72282	2.72112	0.06235	$n=3$	2.72916	2.72746	0.06220
$n=4$	3.35585	3.35472	0.03354	$n=4$	3.36221	3.36108	0.03347

TABLE II. Comparison between numerical and WKB energies for various values of the barrier  $V_0$  and for several low-lying states. All eigenenergies and potentials are measured in the unit of

The resulting WKB energies and those due to the finite difference method are shown in table II. Similar to the previous results, the percentage error decreases with increasing quantum number  $n$ . Moreover, the strength of the potential  $V_0$  is still the parameter determining the number of confined states. However, we notice that the approximated values are slightly less than the numerical ones in this case. For an infinity hard wall of the potential  $V_0$ , the WKB wavefunction  $\Psi_{II}$  satisfying the boundary condition (15) results in the quantisation of WKB energies associated with the half-space linear potential,

$$E = \left[ \frac{3\sqrt{2}}{8} \pi \left( n - \frac{1}{4} \right) \right]^{2/3} \quad \text{for } n = 1, 2, 3, \dots \quad (20)$$

Considering the results shown in tables II and III for each value of  $n$ , we find the WKB calculation does better with increasing  $V_0$ . Unlike the results in the case of the step-harmonic potential, WKB calculation cannot produce exact eigenenergies for  $V_0 = \infty$ .

WKB eigenenergies are then used to calculate WKB wavefunctions in the same way we did before. They are compared with several numerical wavefunctions in Fig 5. As expected, wavefunctions from both methods agree well with each other everywhere except the region around the turning point  $x_2$ . The distribution of WKB eigenstates can be again explained by considering the local momentum  $p(x)$ .

	$V_0 = \infty$		
	E(numerical)	E(WKB)	Percentage Error
$n = 1$	1.16905	1.16013	0.76372
$n = 2$	2.04397	2.04091	0.15017
$n = 3$	2.76028	2.75858	0.06147
$n = 4$	3.39335	3.39223	0.03319

TABLE III. Comparison between numerical and WKB energies associated with the half-space linear potential. All eigenenergies are measured in the unit of  $E_0 = [(2\hbar K)^2/m]^{1/3}$ .

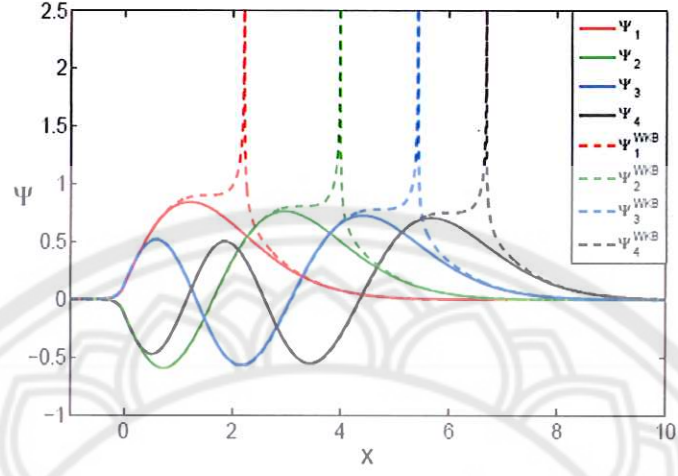


FIG. 5. Comparison between the numerical wavefunctions  $\Psi_n$  and WKB wavefunctions  $\Psi_n^{\text{WKB}}$  corresponding to the step-linear potential with  $V_0 = 50$  for several values of quantum number  $n$ . The distance  $x$  is in the unit of  $a = [\hbar^2/(2Km)]^{1/3}$ .



### 3. วิจารณ์ สรุป และข้อเสนอแนะ

โครงการนี้ได้เสนอวิธีการใช้ WKB สำหรับบ่อพลังงานศักย์ที่มีการเปลี่ยนแปลงอย่างฉับพลันซึ่งประกอบด้วยกำแพงศักย์ที่ตั้งฉากที่จุดวกกลับซึ่งพลังงานศักย์เปลี่ยนแปลงช้า ฟังก์ชันคลื่นจากวิธี WKB มีพฤติกรรมไม่เหมาะสมเพราะการหายไปของโมเมนตัมแต่ในทางตรงกันข้ามอีกจุดวกกลับหนึ่งซึ่งพลังงานศักย์ยกขึ้นอย่างรวดเร็ว ฟังก์ชันคลื่นจากวิธี WKB แสดงพฤติกรรมที่เหมาะสมและคล้ายกับผลจากการคำนวณเชิงตัวเลข เราจึงสามารถเชื่อมฟังก์ชันคลื่นนี้ได้ที่จุดวกกลับนี้ พลังงานที่ได้จากวิธี WKB มีความสอดคล้องกับผลจากการคำนวณเชิงตัวเลขโดยเฉพาะสถานะที่มีพลังงานสูงๆ แม้ว่าการกระจายตัวของ ฟังก์ชันคลื่นจากวิธี WKB จะ ผิดพลาดที่จุดวกกลับซึ่งพลังงานศักย์เปลี่ยนแปลงอย่างช้าๆแต่การกระจายตัวดังกล่าวก็มีความสอดคล้องกับผลจากการคำนวณเชิงตัวเลขในบริเวณที่เหลือเป็นอย่างดี

วิธี WKB ที่พัฒนาขึ้นนี้มีประโยชน์อย่างมาก มันสามารถนำไปประยุกต์ใช้กับพลังงานศักย์ที่ประกอบด้วยกำแพงศักย์ตั้งฉากเช่นพลังงานศักย์แบบสามเหลี่ยมซึ่งพบได้มากที่รอยต่อระหว่างแผ่นสารกึ่งตัวนำสองชนิด ในกรณีของรอยต่อระหว่างสองสารกึ่งตัวนำที่มีความต่างของแถบพลังงานมากๆ วิธี WKB อาจไม่จำเป็นเนื่องจากสามารถประมาณพลังงานศักย์ได้เป็นพลังงานศักย์แบบสามเหลี่ยมที่มีด้านหนึ่งเป็นอนันต์ได้ แต่หากความแตกต่างของแถบพลังงานไม่มากพอ ฟังก์ชันคลื่นจะสามารถทะลุทะลวงเข้าไปในพลังงานศักย์ได้ ทำให้ วิธี WKB ที่พัฒนาขึ้นในงานนี้มีความจำเป็นทันที นอกจากนี้วิธี WKB นี้ยังสามารถนำไปใช้กับสมการชโรดิงเงอร์ในหลายมิติได้อีกเหมือนกับวิธี WKB ทั่วไป แต่ต้องมีการปรับเปลี่ยนปัญหาในหลายมิติให้กลายเป็นปัญหาในหนึ่งมิติเสียก่อน

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## 5. ผลลัพธ์จากโครงการวิจัย

ความรู้ที่ได้จากโครงการวิจัยนี้สามารถนำไปพัฒนาการเรียนการสอนวิชาฟิสิกส์ควอนตัมเรื่องการประมาณ WKB ได้เป็นอย่างดีซึ่งโครงการวิจัยนี้สามารถเขียนบทความเพื่อเผยแพร่ออกมาในวารสารระดับนานาชาติ European Journal of Physics ที่มีค่า Impact Factor 0.619 ได้แก่

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**WKB approximation for abruptly varying potential wells**

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# WKB approximation for abruptly varying potential wells

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(Dated: July 15, 2014)

## Abstract

We present the approach to obtain eigenfunctions and eigenenergies for abruptly varying potentials in the framework of Wentzel-Kramers-Brillouin (WKB) approximation. To illustrate it, two examples of the potentials are studied. The first one is the combination of a step barrier and a harmonic oscillator potential, and the second one consists of a step barrier and a linear potential. The formulation of WKB quantisation rule is proposed. Our approach shows that WKB energies and those from numerical calculation are in good agreement. According to matching conditions used, WKB wavefunctions in this present work are violated at only one classical turning point, but they behave well at another point where the potentials are discontinuous.



## I. INTRODUCTION

The WKB method is a powerful technique for estimating solutions of the Schrödinger equation. Its application is concerned with solving differential equations and can be found in many branches of physics<sup>1-4</sup>. In quantum mechanics classes, students have been taught that WKB approximation is effective when a potential  $V(x)$  changes slowly compared with wavelengths of quantum wavefunctions. This leads to an approximately oscillating wavefunction of the form<sup>5</sup>

$$\Psi(x) = \frac{1}{\sqrt{p(x)}} \exp \left[ \pm \frac{i}{\hbar} \int p(x) dx \right] \quad (1)$$

in a classically allowed region ( $E > V$ ) and an approximately decaying wavefunction of the form

$$\Psi(x) = \frac{1}{\sqrt{|p(x)|}} \exp \left[ \pm \frac{1}{\hbar} \int |p(x)| dx \right] \quad (2)$$

in a classically forbidden region ( $E < V$ ), where  $p(x) = \sqrt{2m[E - V(x)]}$  is the local momentum of a particle with energy  $E$ . Near the turning points where  $E = V$ , WKB wavefunctions do not behave appropriately as the denominators in (1) and (2) go to infinity<sup>6</sup>. As a result, they cannot be matched at the points normally.

To obtain the bound-state energies, the approximated wavefunctions in those two regions are connected by the connection formulae<sup>7</sup> derived by linearising a confined potential well at the turning points. For a potential well which changes slowly, WKB energy quantisation is given by<sup>5,7</sup>

$$\int_{x_1}^{x_2} \sqrt{2m[E_n - V(x)]} dx = \frac{h}{2} \left( n - \frac{1}{2} \right), \quad (3)$$

where  $x_1$  and  $x_2$  are the classical turning points.

The method can also be applied to an abruptly varying potential, particularly a potential with an infinity wall<sup>5,8,9</sup>. In this case, the quantisation energies are obtained by imposing the boundary condition in which the approximated wavefunctions vanish at the infinity wall. Successful examples of the case are an infinity quantum well and a half-space harmonic oscillator (a harmonic oscillator with a hard wall) where WKB approximation gives surprisingly exact eigenenergies<sup>5,9</sup>.

A potential well is not often the case. It could jump upward and then go to a certain value, for instance, a rectangular well formed by a narrower gap semiconductor between two adjacent wider gap semiconductors<sup>10,11</sup>. It seems that the connection formulae do not work



well here because the potential cannot be linearised at the classical turning points. To the best of our knowledge, there is no attempt to apply the WKB method to such a potential.

In this work, we present the approach in the framework of WKB approximation to find the solutions of the Schrödinger equation with a sharply rising potential. To illustrate our idea, we apply the approach to two case studies: the step-harmonic potential<sup>12</sup> (a step barrier and a harmonic oscillator potential) and the step-linear potential<sup>13</sup> (a step barrier and a linear potential). The first one is an interestingly modified harmonic oscillator which could be an exercise in a class. The second one is sometimes called a triangular well which is widely discussed in semiconductor physics<sup>14</sup>. It may be a model for the potential of a heterojunction of two semiconductors with different energy bandgaps. For example, a GaAs-AlGaAs interface<sup>15</sup> where AlGaAs and GaAs are represented by a step and linear barrier respectively. To show the accuracy of our WKB results, we compare them with the eigenenergies and eigenstates obtained by the finite difference method<sup>16</sup>. It is the numerical calculation which can be easily applied to the Schrodinger equitation with any type of confinement potential. Although the highly accurate solutions can be obtained numerically, the solutions are just sets of discretised points. Students may not gain insight into the problems. On the other hand, the WKB theory gives us analytical expression. At least students will understand oscillating and decaying behaviours of quantum wavefunctions. The tendency of allowed energies is also possible to be analysed. The agreement between these two independent methods will be discussed.

## II. WKB ANALYSIS FOR ABRUPTLY VARYING POTENTIALS

We begin this section with the one-dimensional Schrödinger equation:

$$\left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \Psi(x) = E \Psi(x), \quad (4)$$

where  $V(x)$  is a confined potential which rises suddenly at  $x = 0$ . The general model of our considered potential is given by

$$V(x) = \begin{cases} V_1(x) & x < 0 \\ V_2(x) & x \geq 0. \end{cases} \quad (5)$$

$V_1(x)$  and  $V_2(x)$  are arbitrary functions which are not connected each other at  $x = 0$ . In our model, the vertically finite wall is on the side of  $V_1$ , leading to a turning point localised

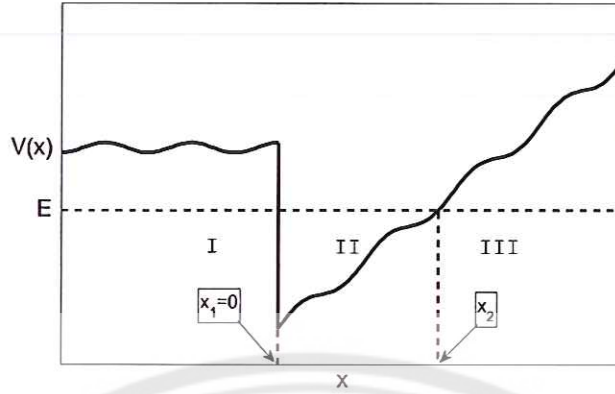


FIG. 1. An attractive potential  $V(x)$  varying abruptly at  $x = 0$ . For a particle with energy  $E$ , the symbols I and III represent the classically forbidden regions, while II represents the classically allowed region.

at  $x_1 = 0$  and another one at  $x_2$  as depicted in Fig. 1. We then express the quantities in the following units:  $x = \tilde{x}a$ ,  $E = \tilde{E}E_0$ , and  $V = \tilde{V}E_0$ , where  $E_0 = \hbar^2/(ma^2)$  and  $a$  is an arbitrary fixed length. Now, the Schrödinger equation (4) becomes

$$\left[ -\frac{1}{2} \frac{\partial^2}{\partial \tilde{x}^2} + \tilde{V}(\tilde{x}) \right] \Psi(\tilde{x}) = \tilde{E} \Psi(\tilde{x}). \quad (6)$$

Note that the tilde will be dropped in the following expression for convenience. It is not a good idea to apply the conventional energy quantisation in equation (3) to our considered potential because of two reasons. Firstly, equation (3) is derived from the assumption that a potential  $V(x)$  depends linearly on the variable  $x$  at the turning points. This assumption is obviously violated at  $x = 0$ . Secondly, integrating from  $x_1$  to  $x_2$  in equation (3) suggests that the approximated eigenenergies are totally independent of the potential in the classically forbidden regions. This is a bad approximation for the investigated potential since  $V_1(x)$ , the potential in region I, indicates how far quantum wavefunctions penetrate into the nonclassical region, and certainly influences the eigenenergies. In other words, it is unreasonable that varying the potential  $V_1(x)$  results in unchanged energies.

We propose that the WKB theory can still be used. The decaying WKB wavefunctions corresponding to the dimensionless Schrödinger equation (6) in the first and the third regions in Fig. 1 are

$$\Psi_I(x) = \frac{A}{\sqrt{\kappa}} \exp \left[ - \int_x^{x_1} \kappa(x') dx' \right] \quad (7)$$



and

$$\Psi_{\text{III}}(x) = \frac{B}{\sqrt{\kappa}} \exp \left[ - \int_{x_2}^x \kappa(x') dx' \right], \quad (8)$$

respectively, where  $A$  and  $B$  are the normalising constants and  $\kappa(x) = \sqrt{2(V - E)}$ . Note that the subscripts refer to the regions where the wavefunctions exist. If  $V_2(x)$  does not change abruptly, we can use the connection formulae to connect the decaying wavefunctions  $\Psi_{\text{III}}$  to the oscillating wavefunctions in region II, obtaining

$$\Psi_{\text{II}}(x) = \frac{2B}{\sqrt{k}} \sin \left[ \int_x^{x_2} k(x') dx' + \frac{\pi}{4} \right], \quad (9)$$

where  $k(x) = \sqrt{2(E - V)}$ . As discussed before, one should not join the wavefunction  $\Psi_{\text{I}}$  and wavefunction  $\Psi_{\text{II}}$  together at  $x = 0$  by using the connection formulae. However, we notice that the WKB wavefunctions in both regions behave well around the turning point  $x = 0$ ; therefore, the wavefunctions can be matched normally by the boundary condition:

$$\left. \frac{\Psi_{\text{I}}'}{\Psi_{\text{I}}} \right|_{x=0} = \left. \frac{\Psi_{\text{II}}'}{\Psi_{\text{II}}} \right|_{x=0}. \quad (10)$$

Now, the coefficients  $A$  and  $B$  are disappeared, and the quantised energies are expected to be obtained after imposing the condition. To demonstrate the advantage of this WKB analysis, we will calculate the eigenenergies and eigenstates associated with the considered potential in the following two examples.

### III. THE STEP-HARMONIC POTENTIAL

The step-harmonic potential which contains a vertically finite wall is of the form discussed in equation (5). It is formed by the step function  $V_0\Theta(-x)$  and the harmonic oscillator potential  $Kx^2\Theta(x)$ , where  $\Theta(x)$  is the Heaviside step function and  $K$  is a constant indicating the width of the quantum well. To get the Schrödinger equation in the dimensionless form of equation (6), we measure energies in the unit of  $E_0 = \hbar^2/(ma^2)$ , where  $a$  is the length  $[\hbar^2/(2Km)]^{1/4}$ . The potential is consequently expressed as

$$V(x) = \begin{cases} V_0 & x < 0 \\ x^2/2 & x \geq 0, \end{cases} \quad (11)$$

as depicted in Fig 2. Before constructing WKB wavefunctions, we need to calculate the



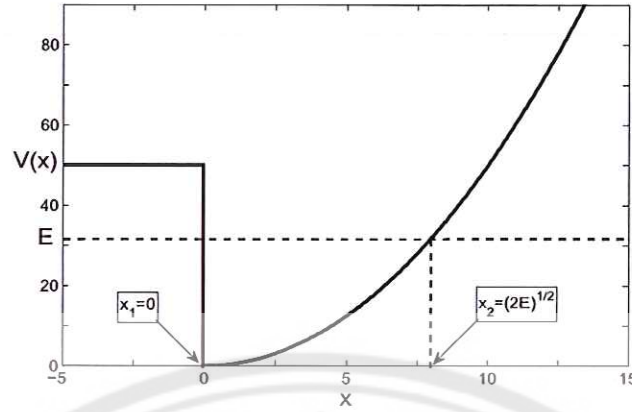


FIG. 2. The step-harmonic potential with the classical turning points at  $x_1 = 0$  and  $x_2 = \sqrt{2E}$ . The potential  $V(x)$  and distance  $x$  are in units of  $E_0 = \hbar \sqrt{\frac{2K}{m}}$  and  $a = \left(\frac{\hbar^2}{2Km}\right)^{1/4}$  respectively.

integrals

$$\begin{aligned} \int_x^{x_1} \kappa(x') dx' &= \int_x^0 \sqrt{2(V_0 - E)} dx' \\ &= -x \sqrt{2(V_0 - E)} \end{aligned} \quad (12)$$

and

$$\begin{aligned} \int_x^{x_2} k(x') dx' &= \int_x^{\sqrt{2E}} \sqrt{2 \left( E - \frac{x'^2}{2} \right)} dx' \\ &= \frac{E\pi}{2} - \left[ \frac{x}{2} \sqrt{2E - x^2} + E \tan^{-1} \left( \frac{x}{\sqrt{2E - x^2}} \right) \right]. \end{aligned} \quad (13)$$

In the above calculation, the classical turning points are localised at  $x_1 = 0$  and  $x_2 = \sqrt{2E}$ . We straightforwardly substitute equations (12) and (13) into the WKB wavefunctions  $\Psi_I$  (7) and  $\Psi_{II}$  (9), then applying the boundary condition (10) to get the energy quantisation rule:

$$\sqrt{V_0 - E} = -\sqrt{E} \cot \theta, \quad (14)$$

where  $\theta = \left( \frac{E\pi}{2} + \frac{\pi}{4} \right)$ .

Our WKB energies are compared with ones from the finite difference method which are converged and accurate to 5 decimal places. Table I shows that WKB energies and those due to the numerical calculation are in very good agreement; the percentage error is less than 0.5 for all trial values of  $V_0$ . We notice that the approximated values are always greater

than the numerical ones. The number of confined states is determined by the strength of the potential  $V_0$ ; it increases as the potential is stronger. For a given value of  $V_0$ , the agreement between two independent methods is improved with increasing  $n$ . That is, the approximation is better for higher energy states. This is the conventional trend in the WKB method, which can be explained by the inspirational assumption that a potential  $V(x)$  changes slowly compared with wavelengths of quantum wavefunctions. In other words, the distance on which a potential changes significantly is large compared with quantum wavelengths. Therefore, high-energy excited states with small wavelengths seem to satisfy the assumption more than the low-lying confined states. For each value of  $n$ , the table shows WKB approximation gives higher accurate results when the potential  $V_0$  is stronger. When the potential  $V_0$  becomes an infinity well, a quantum wavefunction cannot tunnel through the side. In this case, we have the boundary condition

$$\Psi_{II}(x=0) = 0, \quad (15)$$

resulting in the quantised energies

$$E = n - \frac{1}{2} \quad \text{for } n = 2, 4, 6, \dots \quad (16)$$

This is the exact solution of the half-space harmonic oscillator which confirms that WKB calculation is a good approximation for high strength of the barrier  $V_0$ .

After obtaining eigenenergies, we use them to calculate WKB eigenfunctions in those three regions and combine them together to get total WKB wavefunctions ( $\Psi^{\text{WKB}} = \Psi_I + \Psi_{II} + \Psi_{III}$ ). The first 4 eigenstates corresponding to the step-harmonic potential with  $V_0 = 50$  are shown in Fig 3. We find WKB eigenstates have the same behaviour as those from the finite difference method everywhere except the region around the turning point  $x_2$ . They go to infinity at the turning point, but behave very well at another point  $x_1 = 0$ . The local momentum  $p(x)$  plays a key role in the distribution of WKB wavefunctions at the turning points. At  $x_2$  the energies of trapped states are equal to the potential, resulting in  $p(x_2) = 0$  and inappropriate distribution of WKB wavefunctions; on the other hand, at  $x_1$  the quantised energies that are always less than  $V_0$  lead to  $p(x_1) \neq 0$  and appropriate distribution of the wavefunctions.



$V_0=10$				$V_0=50$			
	E(numerical)	E(WKB)	Percentage error		E(numerical)	E(WKB)	Percentage error
$n=1$	1.26217	1.26820	0.47762	$n=1$	1.39055	1.39323	0.19261
$n=2$	3.12085	3.12253	0.05376	$n=2$	3.33290	3.33373	0.02495
$n=3$	4.99927	5.00000	0.01467	$n=3$	5.28869	5.28911	0.00799
$n=4$	6.87711	6.87747	0.00529	$n=4$	7.25102	7.25128	0.00364
$V_0=90$				$V_0=130$			
	E(numerical)	E(WKB)	Percentage error		E(numerical)	E(WKB)	Percentage error
$n=1$	1.41785	1.41983	0.13978	$n=1$	1.43139	1.43304	0.11470
$n=2$	3.37530	3.37592	0.01845	$n=2$	3.39612	3.39664	0.01527
$n=3$	5.34298	5.34330	0.00600	$n=3$	5.36944	5.36971	0.00500
$n=4$	7.31574	7.31594	0.00278	$n=4$	7.34702	7.34719	0.00234

TABLE I. Comparison between numerical and WKB energies for various values of the barrier  $V_0$  and for several low-lying states. All eigenenergies and potentials are measured in the unit of  $E_0 = \hbar\sqrt{\frac{2K}{m}}$ .

#### IV. THE STEP-LINEAR POTENTIAL

The next example we will show is a particle in the step-linear potential. It is the potential with a vertical wall at  $x = 0$ , containing the step function  $V_0\Theta(-x)$  and the linear potential  $Kx\Theta(x)$ , where  $K$  is a constant determining the slope of the linear term. The Schrödinger equation can be written in the dimensionless form of equation (6) by introducing the energy unit  $E_0 = \hbar^2/(ma^2)$ , where  $a = [\hbar^2/(2Km)]^{1/3}$ . Now, the dimensionless potential becomes

$$V(x) = \begin{cases} V_0 & x < 0 \\ x/2 & x \geq 0, \end{cases} \quad (17)$$

where the classical turning points are at  $x_1 = 0$  and  $x_2 = 2E$ , shown in Fig 4. Again, we start finding WKB wavefunctions by calculating the integral

$$\begin{aligned} \int_x^{x_2} k(x')dx' &= \int_x^{2E} \sqrt{2\left(E - \frac{x'}{2}\right)}dx' \\ &= \frac{2}{3}(2E - x)^{3/2}. \end{aligned} \quad (18)$$



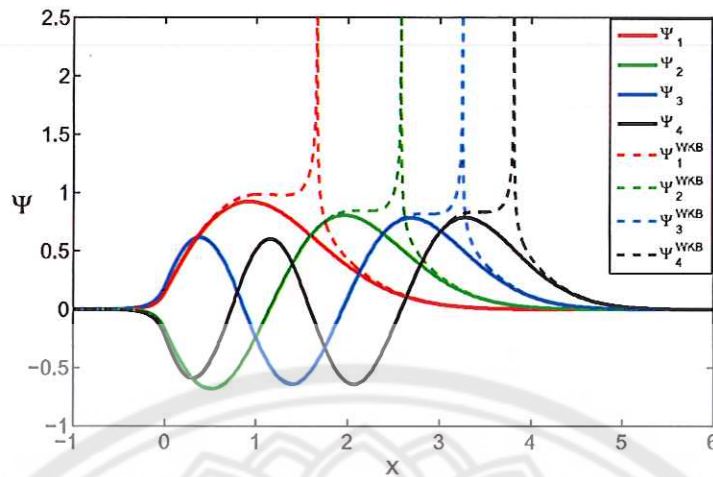


FIG. 3. Comparison between the numerical wavefunctions  $\Psi_n$  and WKB wavefunctions  $\Psi_n^{\text{WKB}}$  corresponding to the step-harmonic potential with  $V_0 = 50$  for several values of quantum number  $n$ . The distance  $x$  is in the unit of  $a = \left(\frac{\hbar^2}{2Km}\right)^{1/4}$ .

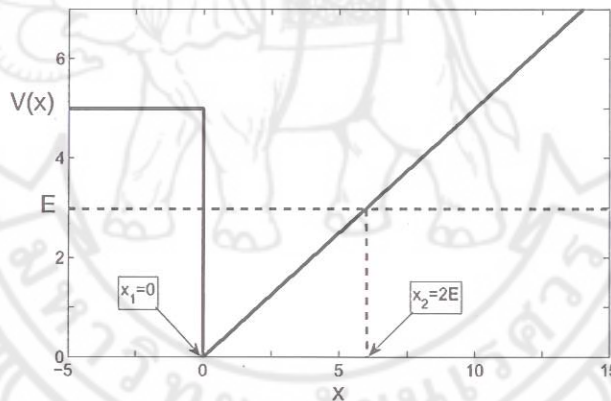


FIG. 4. The step-linear potential with the classical turning points at  $x_1 = 0$  and  $x_2 = 2E$ . The potential  $V(x)$  and distance  $x$  are in units of  $E_0 = [(2\hbar K)^2/m]^{1/3}$  and  $a = [\hbar^2/(2Km)]^{1/3}$  respectively.

Substitute equations (12) and (18) into the WKB wavefunctions  $\Psi_I$  (7) and  $\Psi_{II}$  (9), and impose the boundary condition (10) to obtain the energy quantisation rule:

$$E(V_0 - E)^{1/2} = \frac{\sqrt{2}}{16} - E^{3/2} \cot(\theta), \quad (19)$$

where  $\theta = \frac{4\sqrt{2}}{3}E^{3/2} + \frac{\pi}{4}$ .

The resulting WKB energies and those due to the finite difference method are shown in table II. Similar to the previous results, the percentage error decreases with increasing quantum number  $n$ . Moreover, the strength of the potential  $V_0$  is still the parameter determining the number of confined states. However, we notice that the approximated values are slightly less than the numerical ones in this case. For an infinity hard wall of the potential  $V_0$ , the

$V_0=10$				$V_0=50$			
	E(numerical)	E(WKB)	Percentage error		E(numerical)	E(WKB)	Percentage error
$n=1$	1.05529	1.04625	0.85661	$n=1$	1.11887	1.10993	0.79877
$n=2$	1.92834	1.92524	0.16090	$n=2$	1.99364	1.99057	0.15410
$n=3$	2.64297	2.64126	0.06489	$n=3$	2.70982	2.70812	0.06268
$n=4$	3.27445	3.27331	0.03472	$n=4$	3.34278	3.34166	0.03369
$V_0=90$				$V_0=130$			
	E(numerical)	E(WKB)	Percentage error		E(numerical)	E(WKB)	Percentage error
$n=1$	1.13171	1.12278	0.78924	$n=1$	1.13800	1.12907	0.78474
$n=2$	2.00657	2.00350	0.15302	$n=2$	2.01289	2.00982	0.15252
$n=3$	2.72282	2.72112	0.06235	$n=3$	2.72916	2.72746	0.06220
$n=4$	3.35585	3.35472	0.03354	$n=4$	3.36221	3.36108	0.03347

TABLE II. Comparison between numerical and WKB energies for various values of the barrier  $V_0$  and for several low-lying states. All eigenenergies and potentials are measured in the unit of  $E_0 = [(2\hbar K)^2/m]^{1/3}$ .

WKB wavefunction  $\Psi_{II}$  satisfying the boundary condition (15) results in the quantisation of WKB energies associated with the half-space linear potential,

$$E = \left[ \frac{3\sqrt{2}}{8} \pi \left( n - \frac{1}{4} \right) \right]^{2/3} \quad \text{for } n = 1, 2, 3, \dots \quad (20)$$

Considering the results shown in tables II and III for each value of  $n$ , we find the WKB calculation does better with increasing  $V_0$ . Unlike the results in the case of the step-harmonic potential, WKB calculation cannot produce exact eigenenergies for  $V_0 = \infty$ .

WKB eigenenergies are then used to calculate WKB wavefunctions in the same way we did before. They are compared with several numerical wavefunctions in Fig 5. As expected, wavefunctions from both methods agree well with each other everywhere except the region



	$V_0 = \infty$		
	E(numerical)	E(WKB)	Percentage Error
$n = 1$	1.16905	1.16013	0.76372
$n = 2$	2.04397	2.04091	0.15017
$n = 3$	2.76028	2.75858	0.06147
$n = 4$	3.39335	3.39223	0.03319

TABLE III. Comparison between numerical and WKB energies associated with the half-space linear potential. All eigenenergies are measured in the unit of  $E_0 = [(2\hbar K)^2/m]^{1/3}$ .

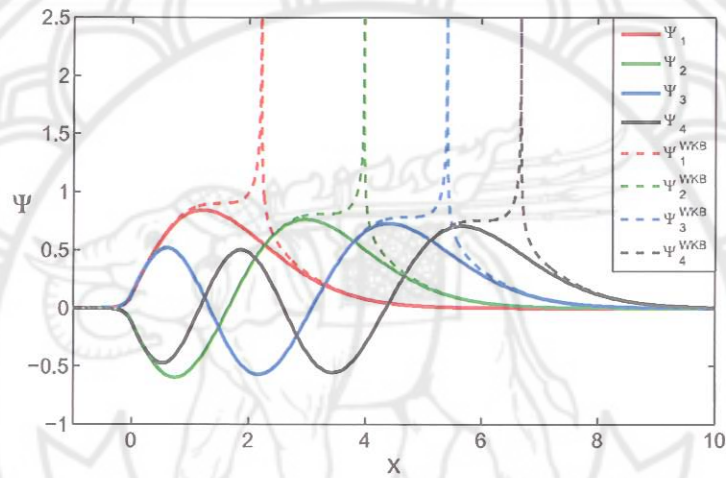


FIG. 5. Comparison between the numerical wavefunctions  $\Psi_n$  and WKB wavefunctions  $\Psi_n^{\text{WKB}}$  corresponding to the step-linear potential with  $V_0 = 50$  for several values of quantum number  $n$ . The distance  $x$  is in the unit of  $a = [\hbar^2/(2Km)]^{1/3}$ .

around the turning point  $x_2$ . The distribution of WKB eigenstates can be again explained by considering the local momentum  $p(x)$ .

## V. CONCLUSION

WKB analysis for abruptly varying potentials containing one vertically finite wall is presented. At the classical turning point where a potential changes slowly, WKB wavefunctions do not behave well because of the vanished momentum. To match WKB wavefunctions at



the point, one needs to use the connection formulae. On the other hand, at another turning point where a potential rises suddenly, WKB wavefunctions exhibit good behaviour. We therefore suggest that the wavefunctions should be matched normally (a quantum wavefunction and its first derivative are continuous at the turning point). Our resulting eigenenergies are found to be in good agreement with the numerical results especially for high-energy excited states. Although WKB eigenstates are violated at the turning point (a quantum wavefunction must be finite everywhere.), their distribution is mostly consistent with that due to the numerical calculation.

Finally, the advantages of our WKB analysis are discussed in the following. It can be applied to the potential with a vertical wall. As seen in our examples, we apply it to a triangular potential which is found at the interface between two layers of different semiconductors<sup>15</sup>. At the conduction band edge, electrons trapped by the potential lead to a two-dimensional electron gas which refers to electrons moving freely in the plane parallel to the interface. For a heterostructure of two semiconductors with a sufficiently large difference of energy band gaps, the half-space linear potential (a linear potential and an infinity wall) may be a good approximation of the confined potential. However, when the energy band gaps are not different enough, quantum wavefunctions can significantly enter into the side of the vertical wall. In this case, our WKB approach is necessary. Moreover, it can be applied to the multidimensional Schrödinger equation with a centrally symmetric potential. Like the standard WKB approach<sup>17,18</sup>, a multidimensional problem is needed to be transformed into the one-dimensional radial equation before applying the WKB method as usual.

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# WKB approximation for abruptly varying potential wells

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## Abstract

We present an approach to obtain eigenfunctions and eigenenergies for abruptly varying potentials in the framework of the Wentzel–Kramers–Brillouin (WKB) approximation. To illustrate it, two examples of the potentials are studied. The first one is the combination of a step barrier and a harmonic oscillator potential, and the second one consists of a step barrier and a linear potential. The formulation of a WKB quantization rule is proposed. Our approach shows that WKB energies and those from numerical calculation are in good agreement. According to matching conditions used, WKB wavefunctions in this present work are violated at only one classical turning point, but they behave well at another point where the potentials are discontinuous.

Keywords: WKB approximation, step-harmonic potential, step-linear potential

## 1. Introduction

The Wentzel–Kramers–Brillouin (WKB) method is a powerful technique for estimating solutions of the Schrödinger equation. Its application is concerned with solving differential equations and can be found in many branches of physics [1–4]. In quantum mechanics classes, students have been taught that WKB approximation is effective when a potential  $V(x)$  changes slowly compared with wavelengths of quantum wavefunctions. This leads to an approximately oscillating wavefunction of the form [5]

$$\Psi(x) = \frac{1}{\sqrt{p(x)}} \exp\left[\pm \frac{i}{\hbar} \int p(x) dx\right] \quad (1)$$

in a classically allowed region ( $E > V$ ) and an approximately decaying wavefunction of the form



$$\Psi(x) = \frac{1}{\sqrt{|p(x)|}} \exp\left[\pm \frac{1}{\hbar} \int |p(x)| dx\right] \quad (2)$$

in a classically forbidden region ( $E < V$ ), where  $p(x) = \sqrt{2m[E - V(x)]}$  is the local momentum of a particle with energy  $E$ . Near the turning points where  $E = V$ , WKB wavefunctions do not behave appropriately as the denominators in (1) and (2) go to infinity [6]. As a result, they cannot be matched at the points normally.

To obtain the bound-state energies, the approximated wavefunctions in those two regions are connected by the connection formulae [7] derived by linearizing a confined potential well at the turning points. For a potential well which changes slowly, WKB energy quantization is given by [5, 7]

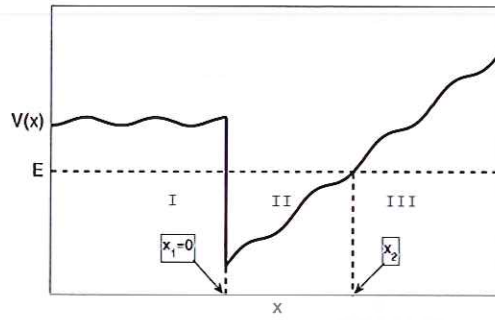
$$\int_{x_1}^{x_2} \sqrt{2m[E_n - V(x)]} dx = \frac{h}{2} \left(n - \frac{1}{2}\right), \quad (3)$$

where  $x_1$  and  $x_2$  are the classical turning points.

The method can also be applied to an abruptly varying potential, particularly a potential with an infinity wall [5, 8, 9]. In this case, the quantization energies are obtained by imposing the boundary condition under which the approximated wavefunctions vanish at the infinity wall. Successful examples of the case are an infinity quantum well and a half-space harmonic oscillator (a harmonic oscillator with a hard wall) where WKB approximation gives surprisingly exact eigenenergies [5, 9].

A potential well is not often the case. It could jump upward and then go to a certain value; for instance, a rectangular well formed by a narrower gap semiconductor between two adjacent wider gap semiconductors [10, 11]. It seems that the connection formulae do not work well here because the potential cannot be linearized at the classical turning points. To the best of our knowledge, there has been no attempt to apply the WKB method to such a potential.

In this work, we present the approach in the framework of the WKB approximation to find the solutions of the Schrödinger equation with a sharply rising potential. To illustrate our idea, we apply the approach to two case studies: the step-harmonic potential [12] (a step barrier and a harmonic oscillator potential) and the step-linear potential [13] (a step barrier and a linear potential). The first one is an interestingly modified harmonic oscillator which could be an exercise in a class. The second one is sometimes called a triangular well which is widely discussed in semiconductor physics [14]. It may be a model for the potential of a heterojunction of two semiconductors with different energy bandgaps; for example, a GaAs-AlGaAs interface [15] where AlGaAs and GaAs are represented by a step and linear barrier respectively. To show the accuracy of our WKB results, we compare them with the eigenenergies and eigenstates obtained by the finite difference method [16]. It is the numerical calculation which can be easily applied to the Schrödinger equation with any type of confinement potential. Although the highly accurate solutions can be obtained numerically, the solutions are just sets of discretized points. Students may not gain insight into the problems. On the other hand, the WKB theory gives us analytical expression. At least students will understand oscillating and decaying behaviours of quantum wavefunctions. The tendency of allowed energies may also be analysed. The agreement between these two independent methods will be discussed.



**Figure 1.** An attractive potential  $V(x)$  varying abruptly at  $x = 0$ . For a particle with energy  $E$ , the symbols I and III represent the classically forbidden regions, while II represents the classically allowed region.

## 2. WKB analysis for abruptly varying potentials

We begin this section with the one-dimensional Schrödinger equation:

$$\left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \Psi(x) = E\Psi(x), \quad (4)$$

where  $V(x)$  is a confined potential which rises suddenly at  $x = 0$ . The general model of our considered potential is given by

$$V(x) = \begin{cases} V_1(x) & x < 0 \\ V_2(x) & x \geq 0. \end{cases} \quad (5)$$

$V_1(x)$  and  $V_2(x)$  are arbitrary functions which are not connected to each other at  $x = 0$ . In our model, the vertically finite wall is on the side of  $V_1$ , leading to a turning point localized at  $x_1 = 0$  and another one at  $x_2$  as depicted in figure 1. We then express the quantities in the following units:  $x = \tilde{x}a$ ,  $E = \tilde{E}E_0$ , and  $V = \tilde{V}E_0$ , where  $E_0 = \hbar^2/(ma^2)$  and  $a$  is an arbitrary fixed length. Now, the Schrödinger equation (4) becomes

$$\left[ -\frac{1}{2} \frac{\partial^2}{\partial \tilde{x}^2} + \tilde{V}(\tilde{x}) \right] \Psi(\tilde{x}) = \tilde{E}\Psi(\tilde{x}). \quad (6)$$

Note that the tilde will be dropped in the following expression for convenience. It is not a good idea to apply the conventional energy quantization in equation (3) to our considered potential for two reasons. Firstly, equation (3) is derived from the assumption that a potential  $V(x)$  depends linearly on the variable  $x$  at the turning points. This assumption is obviously violated at  $x = 0$ . Secondly, integrating from  $x_1$  to  $x_2$  in equation (3) suggests that the approximated eigenenergies are totally independent of the potential in the classically forbidden regions. This is a bad approximation for the investigated potential since  $V_1(x)$ , the potential in region I, indicates how far quantum wavefunctions penetrate into the nonclassical region, and certainly influences the eigenenergies. In other words, it is unreasonable that varying the potential  $V_1(x)$  results in unchanged energies.

We propose that the WKB theory can still be used. The decaying WKB wavefunctions corresponding to the dimensionless Schrödinger equation (6) in the first and the third regions in figure 1 are



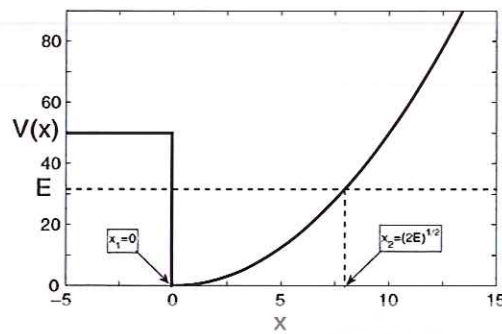


Figure 2. The step-harmonic potential with the classical turning points at  $x_1 = 0$  and  $x_2 = \sqrt{2E}$ . The potential  $V(x)$  and distance  $x$  are in units of  $E_0 = \hbar \sqrt{\frac{2K}{m}}$  and  $a = (\frac{\hbar^2}{2Km})^{1/4}$  respectively.

$$\Psi_I(x) = \frac{A}{\sqrt{\kappa}} \exp\left[-\int_x^{x_1} \kappa(x') dx'\right] \quad (7)$$

and

$$\Psi_{III}(x) = \frac{B}{\sqrt{\kappa}} \exp\left[-\int_{x_2}^x \kappa(x') dx'\right], \quad (8)$$

respectively, where  $A$  and  $B$  are the normalizing constants and  $\kappa(x) = \sqrt{2(V - E)}$ . Note that the subscripts refer to the regions where the wavefunctions exist. If  $V_2(x)$  does not change abruptly, we can use the connection formulae to connect the decaying wavefunctions  $\Psi_{III}$  to the oscillating wavefunctions in region II, obtaining

$$\Psi_{II}(x) = \frac{2B}{\sqrt{k}} \sin\left[\int_x^{x_2} k(x') dx' + \frac{\pi}{4}\right], \quad (9)$$

where  $k(x) = \sqrt{2(E - V)}$ . As discussed before, one should not join together the wavefunction  $\Psi_I$  and wavefunction  $\Psi_{II}$  at  $x = 0$  by using the connection formulae. However, we notice that the WKB wavefunctions in both regions behave well around the turning point  $x = 0$ ; therefore, the wavefunctions can be matched normally by the boundary condition

$$\frac{\Psi'_I}{\Psi_I} \Big|_{x=0} = \frac{\Psi'_{II}}{\Psi_{II}} \Big|_{x=0}. \quad (10)$$

Now, the coefficients  $A$  and  $B$  have disappeared, and the quantized energies are expected to be obtained after imposing the condition. To demonstrate the advantage of this WKB analysis, we will calculate the eigenenergies and eigenstates associated with the considered potential in the following two examples.

### 3. The step-harmonic potential

The step-harmonic potential which contains a vertically finite wall is of the form discussed in equation (5). It is formed by the step function  $V_0\theta(-x)$  and the harmonic oscillator potential  $Kx^2\theta(x)$ , where  $\theta(x)$  is the Heaviside step function and  $K$  is a constant indicating the width of the quantum well. To get the Schrödinger equation in the dimensionless form of



**Table 1.** Comparison between numerical and WKB energies for various values of the barrier  $V_0$  and for several low-lying states. All eigenenergies and potentials are measured in the unit of  $E_0 = \hbar\sqrt{\frac{2K}{m}}$ .

$V_0 = 10$				$V_0 = 50$			
	$E$ (numerical)	$E$ (WKB)	Percentage error		$E$ (numerical)	$E$ (WKB)	Percentage error
$n = 1$	1.26217	1.26820	0.47762	$n = 1$	1.39055	1.39323	0.19261
$n = 2$	3.12085	3.12253	0.05376	$n = 2$	3.33290	3.33373	0.02495
$n = 3$	4.99927	5.00000	0.01467	$n = 3$	5.28869	5.28911	0.00799
$n = 4$	6.87711	6.87747	0.00529	$n = 4$	7.25102	7.25128	0.00364

$V_0 = 90$				$V_0 = 130$			
	$E$ (numerical)	$E$ (WKB)	Percentage error		$E$ (numerical)	$E$ (WKB)	Percentage error
$n = 1$	1.41785	1.41983	0.13978	$n = 1$	1.43139	1.43304	0.11470
$n = 2$	3.37530	3.37592	0.01845	$n = 2$	3.39612	3.39664	0.01527
$n = 3$	5.34298	5.34330	0.00600	$n = 3$	5.36944	5.36971	0.00500
$n = 4$	7.31574	7.31594	0.00278	$n = 4$	7.34702	7.34719	0.00234

equation (6), we measure energies in the unit of  $E_0 = \hbar^2/(ma^2)$ , where  $a$  is the length  $[\hbar^2/(2Km)]^{1/4}$ . The potential is consequently expressed as

$$V(x) = \begin{cases} V_0 & x < 0 \\ x^2/2 & x \geq 0, \end{cases} \quad (11)$$

as depicted in figure 2. Before constructing WKB wavefunctions, we need to calculate the integrals

$$\begin{aligned} \int_x^{x_1} \kappa(x') dx' &= \int_x^0 \sqrt{2(V_0 - E)} dx' \\ &= -x\sqrt{2(V_0 - E)} \end{aligned} \quad (12)$$

and

$$\begin{aligned} \int_x^{x_2} k(x') dx' &= \int_x^{\sqrt{2E}} \sqrt{2\left(E - \frac{x'^2}{2}\right)} dx' \\ &= \frac{E\pi}{2} - \left[ \frac{x}{2} \sqrt{2E - x^2} + E \tan^{-1}\left(\frac{x}{\sqrt{2E - x^2}}\right) \right]. \end{aligned} \quad (13)$$

In the above calculation, the classical turning points are localized at  $x_1 = 0$  and  $x_2 = \sqrt{2E}$ . We straightforwardly substitute equations (12) and (13) into the WKB wavefunctions  $\Psi_I$  (7) and  $\Psi_{II}$  (9), then apply the boundary condition (10) to get the energy quantization rule:

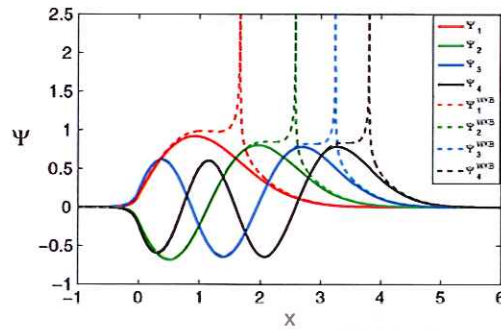


Figure 3. Comparison between the numerical wavefunctions  $\Psi_n$  and WKB wavefunctions  $\Psi_n^{\text{WKB}}$  corresponding to the step-harmonic potential with  $V_0 = 50$  for several values of quantum number  $n$ . The distance  $x$  is in the unit of  $a = (\frac{\hbar^2}{2Km})^{1/4}$ .

$$\sqrt{V_0 - E} = -\sqrt{E} \cot \theta, \quad (14)$$

where  $\theta = \left(\frac{E\pi}{2} + \frac{\pi}{4}\right)$ .

Our WKB energies are compared with ones from the finite difference method which are converged and accurate to five decimal places. Table 1 shows that the WKB energies and those due to the numerical calculation are in very good agreement; the percentage error is less than 0.5 for all trial values of  $V_0$ . We notice that the approximated values are always greater than the numerical ones. The number of confined states is determined by the strength of the potential  $V_0$ ; it increases as the potential becomes stronger. For a given value of  $V_0$ , the agreement between two independent methods is improved with increasing  $n$ . That is, the approximation is better for higher energy states. This is the conventional trend in the WKB method, which can be explained by the inspirational assumption that a potential  $V(x)$  changes slowly compared with wavelengths of quantum wavefunctions. In other words, the distance at which a potential changes significantly is large compared with quantum wavelengths. Therefore, high-energy excited states with small wavelengths seem to satisfy the assumption more than the low-lying confined states. For each value of  $n$ , the table shows that WKB approximation gives higher accurate results when the potential  $V_0$  is stronger. When the potential  $V_0$  becomes an infinity well, a quantum wavefunction cannot tunnel through the side. In this case, we have the boundary condition

$$\Psi_{\text{II}}(x=0) = 0, \quad (15)$$

resulting in the quantized energies

$$E = n - \frac{1}{2} \quad \text{for } n = 2, 4, 6, \dots \quad (16)$$

This is the exact solution of the half-space harmonic oscillator, which confirms that the WKB calculation is a good approximation for the high strength of the barrier  $V_0$ .

After obtaining eigenenergies, we use them to calculate WKB eigenfunctions in those three regions and combine them together to get total WKB wavefunctions ( $\Psi^{\text{WKB}} = \Psi_{\text{I}} + \Psi_{\text{II}} + \Psi_{\text{III}}$ ). The first four eigenstates corresponding to the step-harmonic potential with  $V_0 = 50$  are shown in figure 3. We find WKB eigenstates have the same behaviour as those from the finite difference method everywhere except the region around the turning point  $x_2$ . They go to infinity at the turning point, but behave very well at another point  $x_1 = 0$ . The local momentum  $p(x)$  plays a key role in the distribution of WKB wavefunctions

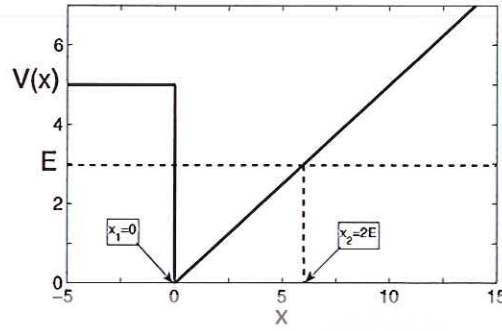


Figure 4. The step-linear potential with the classical turning points at  $x_1 = 0$  and  $x_2 = 2E$ . The potential  $V(x)$  and distance  $x$  are in units of  $E_0 = [(2\hbar K)^2/m]^{1/3}$  and  $a = [\hbar^2/(2Km)]^{1/3}$  respectively.

at the turning points. At  $x_2$ , the energies of trapped states are equal to the potential, resulting in  $p(x_2) = 0$  and inappropriate distribution of WKB wavefunctions; on the other hand, at  $x_1$ , the quantized energies that are always less than  $V_0$  lead to  $p(x_1) \neq 0$  and appropriate distribution of the wavefunctions.

#### 4. The step-linear potential

The next example we will show is a particle in the step-linear potential. It is the potential with a vertical wall at  $x = 0$ , containing the step function  $V_0 \Theta(-x)$  and the linear potential  $Kx\Theta(x)$ , where  $K$  is a constant determining the slope of the linear term. The Schrödinger equation can be written in the dimensionless form of equation (6) by introducing the energy unit  $E_0 = \hbar^2/(ma^2)$ , where  $a = [\hbar^2/(2Km)]^{1/3}$ . Now, the dimensionless potential becomes

$$V(x) = \begin{cases} V_0 & x < 0 \\ x/2 & x \geq 0, \end{cases} \quad (17)$$

where the classical turning points are at  $x_1 = 0$  and  $x_2 = 2E$ , shown in figure 4. Again, we start finding WKB wavefunctions by calculating the integral

$$\begin{aligned} \int_x^{x_2} k(x') dx' &= \int_x^{2E} \sqrt{2\left(E - \frac{x'}{2}\right)} dx' \\ &= \frac{2}{3}(2E - x)^{3/2}. \end{aligned} \quad (18)$$

Substitute equations (12) and (18) into the WKB wavefunctions  $\Psi_I$  (7) and  $\Psi_{II}$  (9), and impose the boundary condition (10) to obtain the energy quantization rule

$$E(V_0 - E)^{1/2} = \frac{\sqrt{2}}{16} - E^{3/2} \cot(\theta), \quad (19)$$

where  $\theta = \frac{4\sqrt{2}}{3}E^{3/2} + \frac{\pi}{4}$ .

The resulting WKB energies and those due to the finite difference method are shown in table 2. Similar to the previous results, the percentage error decreases with increasing quantum number  $n$ . Moreover, the strength of the potential  $V_0$  is still the parameter determining the number of confined states. However, we notice that the approximated values are



**Table 2.** Comparison between numerical and WKB energies for various values of the barrier  $V_0$  and for several low-lying states. All eigenenergies and potentials are measured in the unit of  $E_0 = [(2\hbar K)^2/m]^{1/3}$ .

$V_0 = 10$				$V_0 = 50$			
	$E$ (numerical)	$E$ (WKB)	Percentage error		$E$ (numerical)	$E$ (WKB)	Percentage error
$n = 1$	1.05529	1.04625	0.85661	$n = 1$	1.11887	1.10993	0.79877
$n = 2$	1.92834	1.92524	0.16090	$n = 2$	1.99364	1.99057	0.15410
$n = 3$	2.64297	2.64126	0.06489	$n = 3$	2.70982	2.70812	0.06268
$n = 4$	3.27445	3.27331	0.03472	$n = 4$	3.34278	3.34166	0.03369

$V_0 = 90$				$V_0 = 130$			
	$E$ (numerical)	$E$ (WKB)	Percentage error		$E$ (numerical)	$E$ (WKB)	Percentage error
$n = 1$	1.13171	1.12278	0.78924	$n = 1$	1.13800	1.12907	0.78474
$n = 2$	2.00657	2.00350	0.15302	$n = 2$	2.01289	2.00982	0.15252
$n = 3$	2.72282	2.72112	0.06235	$n = 3$	2.72916	2.72746	0.06220
$n = 4$	3.35585	3.35472	0.03354	$n = 4$	3.36221	3.36108	0.03347

**Table 3.** Comparison between numerical and WKB energies associated with the half-space linear potential. All eigenenergies are measured in the unit of  $E_0 = [(2\hbar K)^2/m]^{1/3}$ .

$V_0 = \infty$			
	$E$ (numerical)	$E$ (WKB)	Percentage error
$n = 1$	1.16905	1.16013	0.76372
$n = 2$	2.04397	2.04091	0.15017
$n = 3$	2.76028	2.75858	0.06147
$n = 4$	3.39335	3.39223	0.03319

slightly less than the numerical ones in this case. For an infinity hard wall of the potential  $V_0$ , the WKB wavefunction  $\Psi_{II}$  satisfying the boundary condition (15) results in the quantization of WKB energies associated with the half-space linear potential,

$$E = \left[ \frac{3\sqrt{2}}{8} \pi \left( n - \frac{1}{4} \right) \right]^{2/3} \quad \text{for } n = 1, 2, 3, \dots \quad (20)$$

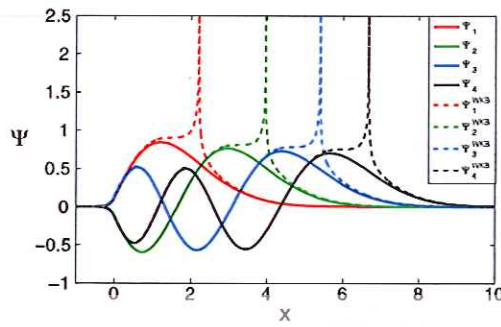


Figure 5. Comparison between the numerical wavefunctions  $\Psi_n$  and WKB wavefunctions  $\Psi_n^{\text{WKB}}$  corresponding to the step-linear potential with  $V_0 = 50$  for several values of quantum number  $n$ . The distance  $x$  is in the unit of  $a = [\hbar^2/(2Km)]^{1/3}$ .

Considering the results shown in tables 2 and 3 for each value of  $n$ , we find the WKB calculation does better with increasing  $V_0$ . Unlike the results in the case of the step-harmonic potential, the WKB calculation cannot produce exact eigenenergies for  $V_0 = \infty$ .

WKB eigenenergies are then used to calculate WKB wavefunctions in the same way we did before. They are compared with several numerical wavefunctions in figure 5. As expected, wavefunctions from both methods agree well with each other everywhere except the region around the turning point  $x_2$ . The distribution of WKB eigenstates can again be explained by considering the local momentum  $p(x)$ .

## 5. Conclusion

WKB analysis for abruptly varying potentials containing one vertically finite wall is presented. At the classical turning point where a potential changes slowly, WKB wavefunctions do not behave well because of the vanished momentum. To match WKB wavefunctions at the point, one needs to use the connection formulae. On the other hand, at another turning point where a potential rises suddenly, WKB wavefunctions exhibit good behaviour. We therefore suggest that the wavefunctions should be matched normally (a quantum wavefunction and its first derivative are continuous at the turning point). Our resulting eigenenergies are found to be in good agreement with the numerical results especially for high-energy excited states. Although WKB eigenstates are violated at the turning point (a quantum wavefunction must be finite everywhere), their distribution is mostly consistent with that due to the numerical calculation.

Finally, the advantages of our WKB analysis are discussed in the following. It can be applied to the potential with a vertical wall. As seen in our examples, we apply it to a triangular potential which is found at the interface between two layers of different semiconductors [15]. At the conduction band edge, electrons trapped by the potential lead to a two-dimensional electron gas which refers to electrons moving freely in the plane parallel to the interface. For a heterostructure of two semiconductors with a sufficiently large difference of energy band gaps, the half-space linear potential (a linear potential and an infinity wall) may be a good approximation of the confined potential. However, when the energy band gaps are not different enough, quantum wavefunctions can significantly enter into the side of the vertical wall. In this case, our WKB approach is necessary. Moreover, it can be applied to the multidimensional Schrödinger equation with a centrally symmetric potential. Like the

standard WKB approach [17, 18], a multidimensional problem needs to be transformed into the one-dimensional radial equation before applying the WKB method as usual.

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