

Problem Statement : WKB approximation

The goal of this problem is to illustrate the full power of the WKB approach, and practice explicitly applying the matching formulae. In undergraduate classes, you likely derived the tunnelling amplitude for specific potentials, e.g. a “top hat” barrier. Now consider a particle with energy E encountering an arbitrary potential barrier $V(x)$:

The classical turning points are located at $x = \alpha$ and $x = \beta$, separating the problem into three regions, 1, 2 and 3. Assuming the WKB approximation holds in every one of these regions, the general solution can be written:

$$\psi_1(x) = \frac{a}{\sqrt{k}} \exp\left(-i \int_x^\alpha k dx\right) + \frac{b}{\sqrt{k}} \exp\left(i \int_x^\alpha k dx\right) \quad (1)$$

$$\psi_2(x) = \frac{c}{\sqrt{\kappa}} \exp\left(-\int_\alpha^x \kappa dx\right) + \frac{d}{\sqrt{\kappa}} \exp\left(\int_\alpha^x \kappa dx\right) \quad (2)$$

$$\psi_3(x) = \frac{f}{\sqrt{k}} \exp\left(i \int_\beta^x k dx\right) + \frac{g}{\sqrt{k}} \exp\left(-i \int_\beta^x k dx\right) \quad (3)$$

1. Use the equations in course notes (Eq 204 to 207) to express that the incoming and outgoing coefficients can be expressed in a neat form,

$$\begin{bmatrix} a \\ b \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 2\theta + \frac{1}{2\theta} & i\left(2\theta - \frac{1}{2\theta}\right) \\ -i\left(2\theta - \frac{1}{2\theta}\right) & 2\theta + \frac{1}{2\theta} \end{bmatrix} \begin{bmatrix} f \\ g \end{bmatrix} \quad (4)$$

where,

$$\theta \equiv \exp\left(\int_\alpha^\beta \kappa(x) dx\right) \quad (5)$$

Hint 1: To start the problem you will first need to put ψ_1 and ψ_3 into the same form as in the matching conditions:

$$2A \cos\left(\int k(x) dx - \frac{\pi}{4}\right) - B \sin\left(\int k(x) dx - \frac{\pi}{4}\right) \quad (6)$$

Determining $A(a, b), B(a, b), A(c, d), B(c, d)$ for e.g. the matching condition at $x = \alpha$ will allow you to express the coefficients as linear functions of each other. Pay special attention to the integral limits.

Hint 2: It is helpful to decompose the problem into two separate transformation matrices,

$$\begin{bmatrix} a \\ b \end{bmatrix} = \mathcal{M}_{cd \rightarrow ab} \mathcal{M}_{fg \rightarrow cd} \begin{bmatrix} f \\ g \end{bmatrix} \quad (7)$$

Solution

Let us write down the equation 204-207 from the lecture notes for reference.

1. Matching a classically accessible region at $x < a$ to a classically inaccessible region $x > a$ (i.e. like the right hand side of the potential well),

$$\frac{2A}{\sqrt{k(x)}} \cos\left(\int_x^a k(x) dx - \frac{\pi}{4}\right) - \frac{B}{\sqrt{k(x)}} \sin\left(\int_x^a k(x) dx - \frac{\pi}{4}\right) \quad (8)$$

should be matched with:

$$\frac{A}{\sqrt{\kappa(x)}} \exp\left(-\int_a^x \kappa(x) dx\right) + \frac{B}{\sqrt{\kappa(x)}} \exp\left(\int_a^x \kappa(x) dx\right) \quad (9)$$

For this problem, such a condition is satisfied when we are going from region I to region II via the α turning point

2. Similarly, when matching a condition for a turning point where $x > b$ is classically accessible region to a classical accessible region $x < b$ (like the left hand side of the potential well)

$$\frac{A}{\sqrt{\kappa(x)}} \exp\left(-\int_x^b \kappa(x) dx\right) + \frac{B}{\sqrt{\kappa(x)}} \exp\left(\int_x^b \kappa(x) dx\right) \quad (10)$$

must be matched with

$$\frac{2A}{\sqrt{k(x)}} \cos\left(\int_b^x k(x) dx - \frac{\pi}{4}\right) - \frac{B}{\sqrt{k(x)}} \sin\left(\int_b^x k(x) dx - \frac{\pi}{4}\right) \quad (11)$$

For our problem such a region is found in going from region II to III via the β turning point

Using the hint, let us put ψ_1 and ψ_3 into the necessary form,

$$\psi_1(x) = \frac{a}{\sqrt{k}} \exp\left(-i \int_x^\alpha k dx\right) + \frac{b}{\sqrt{k}} \exp\left(i \int_x^\alpha k dx\right) \quad (12)$$

$$= \frac{a}{\sqrt{k}} \exp\left(-i \int_x^\alpha k dx + i \frac{\pi}{4}\right) \exp\left(-i \frac{\pi}{4}\right) + \frac{b}{\sqrt{k}} \exp\left(i \int_x^\alpha k dx - i \frac{\pi}{4}\right) \exp\left(i \frac{\pi}{4}\right) \quad (13)$$

$$= \frac{a}{\sqrt{k}} \left(\cos\left(\int_x^\alpha k dx - \frac{\pi}{4}\right) - i \sin\left(\int_x^\alpha k dx - \frac{\pi}{4}\right) \right) \exp\left(-i \frac{\pi}{4}\right) + \frac{b}{\sqrt{k}} \left(\cos\left(\int_x^\alpha k dx - \frac{\pi}{4}\right) + i \sin\left(\int_x^\alpha k dx - \frac{\pi}{4}\right) \right) \exp\left(i \frac{\pi}{4}\right) \quad (14)$$

$$(15)$$

We can match this with A, B from equations 204 and 205 from the notes to get (the A, B from the notes correspond to c, d here).

$$2A = a \exp\left(-i \frac{\pi}{4}\right) + b \exp\left(i \frac{\pi}{4}\right) \quad (16)$$

$$= 2c \quad (17)$$

$$(18)$$

$$B = i \left[a \exp\left(-i \frac{\pi}{4}\right) - b \exp\left(i \frac{\pi}{4}\right) \right] \quad (19)$$

$$= d \quad (20)$$

We can get these two equations above into a matrix form,

$$\begin{bmatrix} c \\ d \end{bmatrix} = \underbrace{\begin{bmatrix} \frac{\exp(-i \frac{\pi}{4})}{2} & \frac{\exp(i \frac{\pi}{4})}{2} \\ i \exp(-i \frac{\pi}{4}) & -i \exp(i \frac{\pi}{4}) \end{bmatrix}}_{\mathcal{M}_{ab \rightarrow cd}} \begin{bmatrix} a \\ b \end{bmatrix} \quad (21)$$

$$(22)$$

Sneak peeking at the question, we can see that we require $\mathcal{M}_{cd \rightarrow ab}$. Computing the inverse of the matrix defined in the above equation will give what we require (Using Mathematica),

$$\mathcal{M}_{cd \rightarrow ab} = \mathcal{M}_{ab \rightarrow cd}^{-1} \quad (23)$$

$$= \begin{bmatrix} \exp(i \frac{\pi}{4}) & -i \frac{\exp(i \frac{\pi}{4})}{2} \\ \exp(-i \frac{\pi}{4}) & i \frac{\exp(-i \frac{\pi}{4})}{2} \end{bmatrix} \quad (24)$$

Now we want to use eq.9 and 10 to find a relationship between A, B and A', B' , where we are defining the primed constants from the equation 10,

$$\frac{A'}{\sqrt{\kappa(x)}} \exp\left(-\int_x^\beta \kappa(x) dx\right) + \frac{B'}{\sqrt{\kappa(x)}} \exp\left(\int_x^\beta \kappa(x) dx\right) \quad (25)$$

We can now break down our integral into two regions where $x \in [\alpha, \beta]$ is broken down into $x \in [x, \beta] = x \in [\alpha, \beta] - x \in [\alpha, x]$

$$= \frac{A'}{\sqrt{\kappa(x)}} \exp \left(- \left[\int_{\alpha}^{\beta} - \int_{\alpha}^x \right] \kappa(x) dx \right) + \frac{B'}{\sqrt{\kappa(x)}} \exp \left(\left[\int_{\alpha}^{\beta} - \int_{\alpha}^x \right] \kappa(x) dx \right) \quad (26)$$

$$= \frac{A'}{\sqrt{\kappa(x)}} \exp \left(- \int_{\alpha}^{\beta} \kappa(x) dx \right) \exp \left(\int_{\alpha}^x \kappa(x) dx \right) + \frac{B'}{\sqrt{\kappa(x)}} \exp \left(\int_{\alpha}^{\beta} \kappa(x) dx \right) \exp \left(- \int_{\alpha}^x \kappa(x) dx \right) \quad (27)$$

We match this with equation 9 given by

$$(205) = \frac{A}{\sqrt{\kappa(x)}} \exp \left(- \int_{\alpha}^x \kappa(x) dx \right) + \frac{B}{\sqrt{\kappa(x)}} \exp \left(\int_{\alpha}^x \kappa(x) dx \right) \quad (28)$$

This gives us,

$$A' = B \exp \left(\int_{\alpha}^{\beta} \kappa(x) dx \right) \quad (29)$$

$$B' = A \exp \left(- \int_{\alpha}^{\beta} \kappa(x) dx \right) \quad (30)$$

We finally need the relationship between A', B' and f, g . We repeat the procedure we did while computing

$$\psi_3(x) = \frac{f}{\sqrt{k}} \exp \left(i \int_{\beta}^x k dx \right) + \frac{g}{\sqrt{k}} \exp \left(-i \int_{\beta}^x k dx \right) \quad (31)$$

$$= \frac{f}{\sqrt{k}} \exp \left(i \frac{\pi}{4} \right) \exp \left(i \left[\int_{\beta}^{\alpha} k dx - \frac{\pi}{4} \right] \right) + \frac{g}{\sqrt{k}} \exp \left(-i \frac{\pi}{4} \right) \exp \left(\left[-i \int_{\beta}^x k dx - \frac{\pi}{4} \right] \right) \quad (32)$$

$$(33)$$

Expanding again in terms of trigonometric functions and comparing A', B' with f, g (Mathematica), we get

$$\mathcal{M}_{fg \rightarrow cd} = \begin{bmatrix} -\theta i \exp \left(i \frac{\pi}{4} \right) & i \theta \exp \left(-i \frac{\pi}{4} \right) \\ \frac{1}{2\theta} \exp \left(i \frac{\pi}{4} \right) & \frac{1}{2\theta} \exp \left(-i \frac{\pi}{4} \right) \end{bmatrix} \quad (34)$$

We can now compute the required "transfer matrix",

$$\mathcal{M}_{fg \rightarrow ab} = \mathcal{M}_{cd \rightarrow ab} \mathcal{M}_{fg \rightarrow cd} \quad (35)$$

$$= \begin{bmatrix} \exp \left(i \frac{\pi}{4} \right) & -i \frac{\exp \left(i \frac{\pi}{4} \right)}{2} \\ \exp \left(-i \frac{\pi}{4} \right) & i \frac{\exp \left(-i \frac{\pi}{4} \right)}{2} \end{bmatrix} \begin{bmatrix} -\theta i \exp \left(i \frac{\pi}{4} \right) & i \theta \exp \left(-i \frac{\pi}{4} \right) \\ \frac{1}{2\theta} \exp \left(i \frac{\pi}{4} \right) & \frac{1}{2\theta} \exp \left(-i \frac{\pi}{4} \right) \end{bmatrix} \quad (36)$$

$$= \frac{1}{2} \begin{bmatrix} 2\theta + \frac{1}{2\theta} & i \left(2\theta - \frac{1}{2\theta} \right) \\ -i \left(\theta - \frac{1}{2\theta} \right) & 2\theta + \frac{1}{2\theta} \end{bmatrix} \quad (37)$$

Which matches the matrix we want to prove in the question.

Solution 1.(b)

$$T = \frac{|\psi_{\text{out}}|^2 V_{\text{out}}}{|\psi_{\text{inc}}|^2 V_{\text{inc}}} \quad (38)$$

$$= \frac{|f|^2}{|a|^2} \quad (39)$$

$$= \frac{|f|^2}{\left| \left(\theta + \frac{1}{4\theta} \right) f \right|^2} \quad (40)$$

$$= \frac{1}{\left| 1 + \frac{1}{4\theta} \right|^2} \quad (41)$$

$$= \frac{1}{\theta^2 \left| 1 + \frac{1}{4\theta^2} \right|^2} \quad (42)$$

$$(43)$$

for $2\theta \ll 1$ we have $\frac{1}{4\theta^2} \approx 0$, giving us $1 + \frac{1}{4\theta}$. Using this we get,

$$T \simeq \theta^{-2} \quad (44)$$

We know,

$$k^2 = \frac{2m}{\hbar} [E - V(x)] \quad (45)$$

that means , k^2 is proportional to velocity. How? It is the difference in the total and the potential energy. And, we are interested in a ratio of two velocities, the constants cancel in the ratio and we can take $v \rightarrow k$.