Calculations for the wave packet through a potential barrier application

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1 Introduction

The aim is to display a wave packet (of wave number k_0 and energy E) passing through a square potential barrier with variable parameters. These are x_{start} and x_{end} where the potential step starts and ends; V_{before}, $V_{barrier}$ and V_{after}, respectively the values of the potential before x_{start}, in between x_{start} and x_{end}, and after x_{end}.

2 Time independent Schrödinger equation

Let's start by calculating the value of the wave function only with the spacial variations (the temporal ones will be calculated later). The stationary Schrödinger equation can be written like this

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \tag{1}$$

To be able to use our parameters we can change the equation by using the wave number value for matter

$$k_0 = \frac{\sqrt{2mE}}{\hbar} \tag{2}$$

By rearranging we get

$$\frac{\hbar^2}{2m} = \frac{E}{{k_0}^2} \tag{3}$$

Replacing it in the Schrödinger equation gives

$$-\frac{E}{{k_0}^2}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \tag{4}$$

Rearranging and simplifying the writing gets us

$$\psi'' + (E - V(x))\frac{{k_0}^2}{E}\psi = 0 \tag{5}$$

By solving this differential equation, you get 3 different equations for $\psi(x)$ depending on the sign of $E - V(x)$

$$\psi(x) = \alpha e^{ikx} + \beta e^{-ikx} \quad \text{if} \quad E - V(x) > 0 \tag{6}$$

$$\psi(x) = \gamma \sinh(Kx) + \lambda \cosh(Kx) \quad \text{if} \quad E - V(x) < 0 \tag{7}$$

$$\psi(x) = \mu x + \sigma \quad \text{if} \quad E - V(x) = 0 \tag{8}$$

with

$$k^2 = (E - V(x))\frac{{k_0}^2}{E} \tag{9}$$

$$K^2 = (V(x) - E)\frac{{k_0}^2}{E} \tag{10}$$

3 Different cases

3.1 $x < x_{start}$

We assume a module of the original wave function of $\alpha = 1$ and we calculate the value ok k_s with Equation 9.

$$\psi(x) = e^{ik_s x} + Re^{-ik_s x} \quad \text{if} \quad E - V_{before} > 0 \tag{11}$$

$$\psi(x) = 0 \quad \text{if} \quad E - V_{before} \leq 0 \tag{12}$$

Where R is the reflection coefficient.

For Equation 12, the energy is smaller or equal to the potential so the packet cannot exist in its starting position.

3.2 $x_{start} \leq x \leq x_{end}$

$$\psi(x) = Ae^{ik_b x} + Be^{-ik_b x} \quad \text{if} \quad E - V_{barrier} > 0 \tag{13}$$

$$\psi(x) = A\sinh(K_b x) + B\cosh(K_b x) \quad \text{if} \quad E - V_{barrier} < 0 \tag{14}$$

$$\psi(x) = Ax + B \quad \text{if} \quad E - V_{barrier} = 0 \tag{15}$$

Where k_b and K_b are the values of k and K calculated from Equation 9 and Equation 10.

3.3 $x > x_{end}$

We assume that the potential stays the same from x_{end} to $+\infty$, so there is no backward component to the wave function ($\beta = \lambda = 0$).

$$\psi(x) = Te^{ik_e x} \quad \text{if} \quad E - V_{after} > 0 \tag{16}$$

$$\psi(x) = T[\cosh(K_e x) - \sinh(K_e x)] = Te^{-K_e x} \quad \text{if} \quad E - V_{after} < 0 \tag{17}$$

$$\psi(x) = T \quad \text{if} \quad E - V_{after} = 0 \tag{18}$$

Where k_e and K_e are the values of k and K calculated from Equation 9 and Equation 10.

Equation 17 has opposites constants because it is the only way for it to tend towards 0 when x approaches ∞.

If we ignore the condition for the calculation of k_e, we can see that $k_e = iK_e$ for $E - V_{after} < 0$. This means that all three equations can be combined to

$$\psi(x) = Te^{ik_e x} \tag{19}$$

3.3.1 Summary of the cases

Firs let's look at Equation 12: from $-\infty$ to x_{start} the value of the wave function is 0. By continuity we can deduce that the wave function is null everywhere.

From there we can see that there are only 3 more cases for $E - V_{before} > 0$ for which the equations to use are:

- (11), (13) and (19) for $E - V_{barrier} > 0$ (subsection 4.1);
- (11), (14) and (19) for $E - V_{barrier} < 0$ (subsection 4.2);
- (11), (15) and (19) for $E - V_{barrier} = 0$ (subsection 4.3);

4 Finding the value of the constants

All constants are found using the continuity of the wave function and its derivative at the boundaries: $\psi_{left}(\chi) = \psi_{right}(\chi)$ and $\psi'_{left}(\chi) = \psi'_{right}(\chi)$. This makes for total of 4 equations with 4 unknowns (2 equations at x_{start} and 2 at x_{end}).

All these cases are calculated with $E - V_{before} \geq 0$ and Equation 11. For simplicity, all notations of x_{start} and x_{end} will be replaced by x_s and x_e.

4.1 Case 1: $E - V_{barrier} > 0$

4.1.1 Continuity at x_{start}

$$(11 = 13) \quad \psi(x_s) = e^{ik_s x_s} + Re^{-ik_s x_s} = Ae^{ik_b x_s} + Be^{-ik_b x_s} \tag{20}$$

$$\Leftrightarrow \boxed{R = e^{ik_s x_s}(Ae^{ik_b x_s} + Be^{-ik_b x_s} - e^{ik_s x_s})} \tag{21}$$

$$(11' = 13') \quad \psi'(x_s) = ik_s e^{ik_s x_s} - ik_s Re^{-ik_s x_s} = ik_b Ae^{ik_b x_s} - ik_b Be^{-ik_b x_s} \tag{22}$$

$$\Leftrightarrow \frac{k_s}{k_b}(e^{ik_s x_s} - Re^{-ik_s x_s}) = Ae^{ik_b x_s} - Be^{-ik_b x_s} \tag{23}$$

Let's set $\boxed{D = \frac{k_s}{k_b}}$ and $\boxed{E = e^{ix_s}}$. Equation 20 becomes

$$E^{k_s} + \frac{R}{E^{k_s}} = AE^{k_b} + \frac{B}{E^{k_b}} \tag{24}$$

And Equation 23 becomes

$$D(E^{k_s} - \frac{R}{E^{k_s}}) = AE^{k_b} - \frac{B}{E^{k_b}} \tag{25}$$

$$\Leftrightarrow E^{k_s} - \frac{R}{E^{k_s}} = \frac{A}{D}E^{k_b} - \frac{B}{DE^{k_b}} \tag{26}$$

From there, Equation 24 can be added to Equation 26

$$2E^{k_s} = (1 + \frac{1}{D})AE^{k_b} + (1 - \frac{1}{D})\frac{B}{E^{k_b}} \tag{27}$$

$$\Leftrightarrow \frac{B}{E^{k_b}}(1 - \frac{1}{D}) = 2E^{k_s} - (1 + \frac{1}{D})AE^{k_b} \tag{28}$$

$$\Leftrightarrow B = \frac{E^{k_b}}{1 - 1/D}[2E^{k_s} - (1 + \frac{1}{D})AE^{k_b}] \tag{29}$$

And replacing the values of D and E gets us

$$\boxed{B = \frac{e^{ik_b x_s}}{1 - k_b/k_s}[2e^{ik_s x_s} - (1 + \frac{k_b}{k_s})Ae^{ik_b x_s}]} \tag{30}$$

4.1.2 Continuity at x_{end}

$$(13 = 19) \quad \psi(x_e) = Ae^{ik_b x_e} + Be^{-ik_b x_e} = Te^{ik_e x_e} \tag{31}$$

$$\Leftrightarrow \boxed{T = e^{-ik_e x_e}(Ae^{ik_b x_e} + Be^{-ik_b x_e})} \tag{32}$$

$$(13' = 19') \quad \psi'(x_e) = ik_b Ae^{ik_b x_e} - ik_b Be^{-ik_b x_e} = ik_e Te^{ik_e x_e} \tag{33}$$

$$\frac{k_b}{k_e}(Ae^{ik_b x_e} - Be^{-ik_b x_e}) = Te^{ik_e x_e} \tag{34}$$

Let's set $\boxed{F = e^{ix_e}}$ and $\boxed{G = \frac{k_b}{k_e}}$. Equation 31 becomes

$$AF^{k_b} + \frac{B}{F^{k_b}} = TF^{k_e} \tag{35}$$

And Equation 34 becomes

$$G(AF^{k_b} - \frac{B}{F^{k_b}}) = TF^{k_e} \tag{36}$$

Subtracting Equation 35 from Equation 36 gives

$$(1 - G)(AF^{k_b} - \frac{B}{F^{k_b}}) = 0 \tag{37}$$

$$\Leftrightarrow B = AF^{2k_b} \tag{38}$$

Replacing with the value of F gets us

$$\boxed{B = Ae^{2ik_b x_e}} \tag{39}$$

4.1.3 Solving x_{start} and x_{end} together

Equaling the values of B in Equation 29 and Equation 38 gives this equation

$$B = \frac{E^{k_b}}{1-1/D}[2E^{k_s} - (1+\frac{1}{D})AE^{k_b}] = AF^{2k_b} \tag{40}$$

$$\Leftrightarrow \frac{2E^{k_s k_b}}{1-1/D} = AF^{2k_b} + \frac{1+1/D}{1-1/D}AE^{2k_b} \tag{41}$$

$$\Leftrightarrow A = \frac{1}{F^{2k_b} + \frac{1+1/D}{1-1/D}E^{2k_b}} \frac{2E^{k_s k_b}}{1-1/D} \tag{42}$$

Replacing the values for D, E and F gives the final result for A, from which the values for B, R and T can be deduced.

$$\boxed{A = \frac{1}{e^{2ik_b x_e} + \frac{1+k_b/k_s}{1-k_b/k_s}e^{2ik_b x_s}} \frac{2e^{ik_s k_b x_s}}{1-k_b/k_s}} \tag{43}$$

4.1.4 Summary of the values for R, T, A and B

$$\boxed{A = \frac{1}{e^{2ik_b x_e} + \frac{1+k_b/k_s}{1-k_b/k_s}e^{2ik_b x_s}} \frac{2e^{ik_s k_b x_s}}{1-k_b/k_s}} \tag{44}$$

$$\boxed{B = Ae^{2ik_b x_e}} \tag{45}$$

$$\boxed{R = e^{ik_s x_s}(Ae^{ik_b x_s} + Be^{-ik_b x_s} - e^{ik_s x_s})} \tag{46}$$

$$\boxed{T = e^{-ik_e x_e}(Ae^{ik_b x_e} + Be^{-ik_b x_e})} \tag{47}$$

4.2 Case 2: $E - V_{barrier} < 0$

4.2.1 Continuity at x_{start}

$$(11 = 14) \quad \psi(x_s) = e^{ik_s x_s} + Re^{-ik_s x_s} = A\sinh(K_b x_s) + B\cosh(K_b x_s) \tag{48}$$

$$(11' = 14') \quad \psi'(x_s) = ik_s e^{ik_s x_s} - ik_s Re^{-ik_s x_s} = AK_b\cosh(K_b x_s) + BK_b\sinh(K_b x_s) \tag{49}$$

4.2.2 Continuity at x_{end}

$$(14 = 19) \quad \psi(x_e) = A\sinh(K_b x_e) + B\cosh(K_b x_e) = Te^{ik_e x_e} \tag{50}$$

$$(14' = 19') \quad \psi'(x_e) = AK_b\cosh(K_b x_e) + BK_b\sinh(K_b x_e) = ik_e Te^{ik_e x_e} \tag{51}$$

4.2.3 Solving x_{start} and x_{end} together

4.2.4 Summary of the values for R, T, A and B

4.3 Case 3: $E - V_{barrier} = 0$

4.3.1 Continuity at x_{start}

$$(11 = 15) \quad \psi(x_s) = e^{ik_s x_s} + Re^{-ik_s x_s} = Ax_s + B \tag{52}$$

$$(11' = 15') \quad \psi'(x_s) = ik_s e^{ik_s x_s} - ik_s Re^{-ik_s x_s} = A \tag{53}$$

4.3.2 Continuity at x_{end}

$$(15 = 19) \quad \psi(x_e) = Ax_e + B = Te^{ik_e x_e} \tag{54}$$

$$(15' = 19') \quad \psi'(x_e) = A = ik_e Te^{ik_e x_e} \tag{55}$$

4.3.3 Solving x_{start} and x_{end} together

4.3.4 Summary of the values for R, T, A and B