Recitation and individual homework 4
Quantum Leakage
Solution

In the recitation we will provide outlines to the solution, while you will complete the homework working alone. You will be graded on a coarse scale, with 0, 5, 10 or 15 marks. Solution will be provided after the deadline, Monday 6 May, 10 am. I find it important you do this assignment on your own to obtain a good working knowledge of Schrodinger mechanics.

Consider the potential energy barrier of length $L$ and height $V_0$ as shown above. An electron is injected from the left. It has energy $E < V_0$.

(a) Write down the wavefunctions in regions I, II and III. These wavefunctions should include physically plausible terms. The Schrodinger equation (space part) is,

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

Answer (a):

The time independent Schrodinger equation is,

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

For Region I:

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For region I the Schrodinger equation, with $V = 0$, is,

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

$$\frac{d^2 \psi(x)}{dx^2} + \frac{2mE}{\hbar^2} \psi(x) = 0$$

$$(D^2 + k^2)\psi(x) = 0,$$  

(1)

where $k = \frac{2mE}{\hbar^2}$.

$$\Rightarrow D^2 = -k^2$$

$$D = \pm ik,$$

which leads to the solution,

$$\psi(x) = Ae^{ikx} + Be^{-ikx}.$$  

the first term on the right is a forward propagating wave and the second term is a backward propagating wave.

**For Region II**: $V = V_0$ and $E < V_0$

The Schrodinger equation for this region becomes,

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + (V_0 - E)\psi(x) = 0$$

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + (V_0 - E)\right)\psi(x) = 0$$

$$\left(\frac{d^2}{dx^2} - \frac{2m}{\hbar^2}(V_0 - E)\right)\psi(x) = 0$$

$$(D^2 - \alpha^2)\psi(x) = 0$$

$$D = \pm \alpha,$$

where $\alpha^2 = \frac{2m(V_0 - E)}{\hbar^2}$, is a positive constant.

Hence wave function for region II is,

$$\psi_{II}(x) = Ce^{\alpha x} + De^{-\alpha x}$$  

(2)

Since the exponents $\alpha$ are real, $\psi_{II}(x)$ does not represent an oscillatory function, rather it is a decreasing function.

Date: 26 April, 2013
For Region III: V=0

Since the wavevector of region III is same as that of region I, hence the solution becomes,

$$\psi(x) = E e^{ikx} + F e^{-ikx}.$$ 

Since the wave does not seen any obstacle in region III, it cannot be reflected implying $F = 0$. The wavefunction therefore, is,

$$\psi_{III}(x) = E e^{ikx}.$$ 

(b) Write down the boundary conditions at $x = 0$ and $x = L$.

**Answer (b):**

The boundary condition at the edges of the barrier are that $\psi(x)$ and $\frac{d\psi(x)}{dx}$ must be continuous at both edges.

**At x=0:**

$$\psi_I(x = 0) = \psi_{III}(x = 0)$$

$$\Rightarrow A + B = C + D$$

and

$$\frac{d\psi_I}{dx} \bigg|_{x=0} = \frac{d\psi_{III}}{dx} \bigg|_{x=0}$$

$$ikA - ikB = \alpha C - \alpha D$$

$$ik(A - B) = \alpha (C - D)$$

$$A - B = -i \frac{\alpha}{k} (C - D).$$

**At x=L:**

$$\psi_{II}(x = L) = \psi_{III}(x = L)$$

$$\Rightarrow Ce^{\alpha L} + De^{-\alpha L} = E e^{ikL}$$

and

$$\frac{d\psi_{II}}{dx} \bigg|_{x=L} = \frac{d\psi_{III}}{dx} \bigg|_{x=L}$$

$$\alpha Ce^{ikL} - \alpha De^{-\alpha L} = ik E e^{ikL}$$

$$Ce^{\alpha L} - De^{-\alpha L} = i \frac{\alpha}{k} e^{ikL}$$

Equations (3), (4), (5) and (6) are the required boundary conditions.
(c) If a single electron is injected, will it be reflected from the wall at \( x = 0 \)? Can it penetrate through the obstacle and be found at \( x > L \)?

**Answer (c):**

If a single electron is injected with energy less than the barrier height \((E < V_0)\), classically the particle cannot penetrate through the barrier, it will be reflected completely. However quantum mechanics tell us that the particle has certain probability to go through the barrier, and this is when the transmission coefficient is non-zero.

(d) Can the electron be “really”—I mean physically be found inside the region II? Use the uncertainty principle to answer this question.

**Answer (d):**

In region II the total energy is less than the potential energy, which means that the particle appears to possess negative kinetic energy here. From equation (2) on page 3, \( 1/\alpha \) represents a penetrating length \( \delta \),

\[
\delta = \frac{1}{\alpha} = \frac{\hbar}{\sqrt{2m(V_0 - E)}},
\]

which characterizes a realm of possibilities of position \( \Delta x \). Now using the uncertainty principle \( \Delta x \Delta p \sim \hbar \)

\[
\Delta p \sim \frac{\hbar \sqrt{2m(V_0 - E)}}{\hbar} = \sqrt{2m(V_0 - E)} \sim p.
\]

The momentum \( p \) corresponds to an energy \( \frac{p^2}{2m} = V_0 - E \) and if we assume that the uncertainty in energy \( \Delta E \) is of the same order as the energy, the \( \Delta E \sim V_0 - E \).

As you immediately recognize, \( V_0 - E \) is of the same order as the energy gap that localizes the particle to the region \( \delta \). If the uncertainty is as large as the gap, there is no guarantee that the particle can be localized.

(e) Find the probability \( T \) that the incident electron from the far left is transmitted into region III.

**Answer (e):**
Transmission probability $T$ is given by,

$$T = \frac{\text{Prob. that the particle crosses right boundary per unit time}}{\text{Prob. that the particle crosses left boundary per unit time}}$$

$$= \frac{|\text{prob/time}|_{x=L}}{|\text{prob/time}|_{x=0}}$$

$$= \frac{|\text{prob/length \times length/time}|_{x=L}}{|\text{prob/length \times length/time}|_{x=0}}$$

$$= \frac{|\psi(x)|^2_{x=L} \times v}{|\psi(x)|^2_{x=0} \times v}$$

$$= \frac{|\psi(x)|^2_{x=L}}{|\psi(x)|^2_{x=0}}.$$

In the given case, $|\psi(x)|^2_{x=L} = |E|^2$ and $|\psi(x)|^2_{x=0} = |A|^2$. Therefore transmission probability is,

$$T = \frac{|E|^2}{|A|^2}.$$

In order to calculate $|E|^2$ and $|A|^2$ we will use the four boundary conditions derived in part (b). Add equation (3) and (4),

$$2A = C \left(1 - i \frac{\alpha}{k}\right) + D \left(1 + i \frac{\alpha}{k}\right)$$

$$A = \frac{C}{2} \left(1 - i \frac{\alpha}{k}\right) + \frac{D}{2} \left(1 + i \frac{\alpha}{k}\right). \quad (7)$$

Next adding equation (5) and (6) we obtain,

$$2Ce^{\alpha L} = E e^{i k L} \left(1 + i \frac{k}{\alpha}\right)$$

$$C = \frac{E e^{i k L}}{2e^{\alpha L}} \left(1 + i \frac{k}{\alpha}\right). \quad (8)$$

Now subtracting equation (6) from (5) results in,

$$2De^{-\alpha L} = E e^{i k L} \left(1 - i \frac{k}{\alpha}\right)$$

$$D = \frac{E e^{i k L}}{2e^{-\alpha L}} \left(1 - i \frac{k}{\alpha}\right). \quad (9)$$

Using values of $C$ and $D$ from equations (8) and (9) in equation (7) yields,

$$A = \frac{1}{2} \left(\frac{E e^{i k L}}{2e^{\alpha L}}\right) \left(1 + i \frac{k}{\alpha}\right) \left(1 - i \frac{\alpha}{k}\right) + \frac{1}{2} \left(\frac{E e^{i k L}}{2e^{-\alpha L}}\right) \left(1 - i \frac{k}{\alpha}\right) \left(1 + i \frac{\alpha}{k}\right)$$

$$= \frac{E e^{i k L}}{4} \left[e^{-\alpha L} \left(1 + i \frac{k}{\alpha} - i \frac{\alpha}{k} + 1\right) + e^{\alpha L} \left(1 + i \frac{\alpha}{k} - i \frac{k}{\alpha} + 1\right)\right]$$

$$= \frac{E e^{i k L}}{4} \left[e^{-\alpha L} \left(2 + i \frac{(k^2 - \alpha^2)}{k\alpha}\right) + e^{\alpha L} \left(2 - i \frac{(k^2 - \alpha^2)}{k\alpha}\right)\right].$$
and after some further rearrangement,

\[ A = \frac{E e^{ikL}}{4} \left[ 2(e^{\alpha L} + e^{-\alpha L}) + i \left( \frac{\alpha^2 - k^2}{k\alpha} \right) (e^{\alpha L} - e^{-\alpha L}) \right] \]

\[ = E e^{ikL} \left[ \left( \frac{e^{\alpha L} + e^{-\alpha L}}{2} \right) + i \left( \frac{\alpha^2 - k^2}{2k\alpha} \right) \left( \frac{e^{\alpha L} - e^{-\alpha L}}{2} \right) \right]. \]

Using \( \cosh x = \frac{e^x + e^{-x}}{2} \) and \( \sinh x = \frac{e^x - e^{-x}}{2} \),

\[ A = E e^{ikL} \left( \cosh(\alpha L) + i \frac{(\alpha^2 - k^2)}{2k\alpha} \sinh(\alpha L) \right). \tag{10} \]

Now taking the complex conjugate of equation (10),

\[ A^* = E^* e^{-ikL} \left( \cosh(\alpha L) - i \frac{(\alpha^2 - k^2)}{2k\alpha} \sinh(\alpha L) \right), \tag{11} \]

and finally multiplying equations (10) and (11) yields,

\[ A^* A = \frac{E^* e^{-ikL}}{4} \left[ 2(e^{\alpha L} + e^{-\alpha L}) - i \left( \frac{\alpha^2 - k^2}{k\alpha} \right) (e^{\alpha L} - e^{-\alpha L}) \right] \cdot E e^{ikL} \left[ \left( \frac{e^{\alpha L} + e^{-\alpha L}}{2} \right) + i \left( \frac{\alpha^2 - k^2}{2k\alpha} \right) \left( \frac{e^{\alpha L} - e^{-\alpha L}}{2} \right) \right]. \]

\[ \left| A \right|^2 = |E|^2 \left( \cosh^2(\alpha L) + \frac{(\alpha^2 - k^2)^2}{4k^2\alpha^2} \sinh^2(\alpha L) \right) \]

\[ = 1 + \sinh^2(\alpha L) + \frac{(\alpha^2 - k^2)^2}{4k^2\alpha^2} \sinh^2(\alpha L) \]

\[ = 1 + \frac{(\alpha^2 + k^2)^2}{4k^2\alpha^2} \sinh^2(\alpha L). \]

Substitute values of \( k \) and \( \alpha \) we obtain the desired result.

\[ \frac{|A|^2}{|E|^2} = T^{-1} = 1 + \frac{(\frac{2m(V_0 - E)}{\hbar^2} + \frac{2mE}{\hbar^2})^2}{4\left(\frac{2m(V_0 - E)}{\hbar^2}\right) \times \left(\frac{2mE}{\hbar^2}\right)} \sinh^2 \left( \frac{L}{\hbar} \sqrt{2m(V_0 - E)} \right) \]

\[ T^{-1} = 1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2 \left( \frac{L}{\hbar} \sqrt{2m(V_0 - E)} \right) \]

\[ T = \left[ 1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2 \left( \frac{L}{\hbar} \sqrt{2m(V_0 - E)} \right) \right]^{-1}. \]
Shown is a graph of $T$ versus $E$ for $V_0 = 10 \times 1.6 \times 10^{-19} \text{ J} = 10 \text{ eV}$ and $E$ in the range of 0 to $30 \times 1.6 \times 10^{-19} \text{ J} (= 30 \text{ eV})$. The length of the barrier $L$ is chosen as 1Å. Clearly as $E$ increases, the transmission $T$ goes up.

(f) Now consider the Fig. (b) with, $E < V_0, \quad E > W_0,$ and $V_0 > W_0$.

Using your result for part (e), find the transmission probability into region III.

**Answer (f):**

Wave functions for the three regions are,

\[
\psi_I(x) = Ae^{ikx} + Be^{-ikx}, \quad \text{where} \quad k = \frac{\sqrt{2mE}}{\hbar}
\]

\[
\psi_{II}(x) = Ce^{\alpha x} + De^{-\alpha x}, \quad \text{where} \quad \alpha = \frac{\sqrt{2m(V_0 - E)}}{\hbar}
\]

\[
\psi_{III}(x) = Ee^{i\beta x}, \quad \text{where} \quad \beta = \frac{\sqrt{2m(E - W_0)}}{\hbar}
\]
The boundary conditions at $x = 0$ are,
\[
\psi_I(0) = \psi_{II}(0)
\]
\[
A + B = C + D \tag{12}
\]
and \[
\psi'_I(0) = \psi'_{II}(0)
\]
\[
A - B = -i \frac{\alpha}{k}(C - D), \tag{13}
\]
while the boundary conditions at $x = L$ are,
\[
\psi_{II}(L) = \psi_{III}(L)
\]
\[
Ce^{\alpha L} + De^{-\alpha L} = Ee^{i\beta L} \tag{14}
\]
and \[
\psi'_{II}(L) = \psi'_{III}(L)
\]
\[
Ce^{\alpha x} - De^{-\alpha L} = i \frac{\beta}{\alpha} Ee^{i\beta L}. \tag{15}
\]
Adding equations (12) and (13),
\[
2A = C \left(1 - i \frac{\alpha}{k}\right) + D \left(1 + i \frac{\alpha}{k}\right)
\]
\[
A = \frac{C}{2} \left(1 - i \frac{\alpha}{k}\right) + \frac{D}{2} \left(1 + i \frac{\alpha}{k}\right), \tag{16}
\]
and add equation (14) and (15),
\[
2Ce^{\alpha L} = Ee^{i\beta L} \left(1 + i \frac{\beta}{\alpha}\right)
\]
\[
C = \frac{Ee^{i\beta L}}{2e^{\alpha L}} \left(1 + i \frac{\beta}{\alpha}\right). \tag{17}
\]
Now subtract equation (15) from (14) we get,
\[
2De^{-\alpha L} = Ee^{i\beta L} \left(1 - i \frac{\beta}{\alpha}\right)
\]
\[
D = \frac{Ee^{i\beta L}}{2e^{-\alpha L}} \left(1 - i \frac{\beta}{\alpha}\right). \tag{18}
\]
Inserting values of $C$ and $D$ from equations (17) and (18) into equation (16) results in,
\[
A = \frac{1}{2} \left(\frac{Ee^{i\beta L}}{2e^{\alpha L}}\right) \left(1 + i \frac{\beta}{\alpha}\right) \left(1 - i \frac{\alpha}{k}\right) + \frac{1}{2} \left(\frac{Ee^{i\beta L}}{2e^{-\alpha L}}\right) \left(1 - i \frac{\beta}{\alpha}\right) \left(1 + i \frac{\alpha}{k}\right)
\]
\[
= \frac{Ee^{i\beta L}}{4} \left[ e^{-\alpha L} \left(1 + i \frac{\beta}{\alpha} - i \frac{\alpha}{k} + \frac{\beta}{k}\right) + e^{\alpha L} \left(1 + i \frac{\alpha}{k} - i \frac{\beta}{\alpha} + \frac{\beta}{k}\right) \right]
\]
\[
= \frac{Ee^{i\beta L}}{4} \left[ e^{-\alpha L} \left(1 + \frac{\beta}{k}\right) + i \left(\frac{\beta}{\alpha} - \frac{\alpha}{k}\right) \right] + e^{\alpha L} \left(1 + \frac{\beta}{k} - i \left(\frac{\beta}{\alpha} - \frac{\alpha}{k}\right) \right)
\]
\[
= \frac{Ee^{i\beta L}}{4} \left[ e^{-\alpha L} \left(1 + \frac{\beta}{k}\right) + ie^{-\alpha L} \left(\frac{\beta}{\alpha} - \frac{\alpha}{k}\right) + e^{\alpha L} \left(1 + \frac{\beta}{k} - i e^{\alpha L} \left(\frac{\beta}{\alpha} - \frac{\alpha}{k}\right) \right) \right].
\]
and after some rearrangement,

\[
A = \frac{E e^{i\beta L}}{4} \left[ (e^{\alpha L} + e^{-\alpha L}) \left( 1 + \frac{\beta}{k} \right) - i(e^{\alpha L} - e^{-\alpha L}) \left( \frac{\beta}{\alpha} - \frac{\alpha}{k} \right) \right] = \frac{E e^{i\beta L}}{2} \left[ \left( \frac{e^{\alpha L} + e^{-\alpha L}}{2} \right) \left( 1 + \frac{\beta}{k} \right) - i \left( \frac{e^{\alpha L} - e^{-\alpha L}}{2} \right) \left( \frac{\beta}{\alpha} - \frac{\alpha}{k} \right) \right].
\]

Using \( \cosh x = \frac{e^x + e^{-x}}{2} \) and \( \sinh x = \frac{e^x - e^{-x}}{2} \),

\[
A = \frac{E e^{i\beta L}}{2} \left[ \cosh(\alpha L) \left( 1 + \frac{\beta}{k} \right) - i \sinh(\alpha L) \left( \frac{\beta}{\alpha} - \frac{\alpha}{k} \right) \right]. \tag{19}
\]

Taking the complex conjugate of equation (19),

\[
A^* = \frac{E^* e^{-i\beta L}}{2} \left[ \cosh(\alpha L) \left( 1 + \frac{\beta}{k} \right) + i \sinh(\alpha L) \left( \frac{\beta}{\alpha} - \frac{\alpha}{k} \right) \right]. \tag{20}
\]

Multiply equations (19) and (20) yields,

\[
|A|^2 = \frac{|E|^2}{4} \left[ \cosh^2(\alpha L) \left( 1 + \frac{\beta}{k} \right)^2 + \sinh^2(\alpha L) \left( \frac{\beta}{\alpha} - \frac{\alpha}{k} \right)^2 \right] = \frac{1}{T}.
\]

If we would like to express the final result explicitly in terms of the energy and length, we obtain. Substitute values of \( k, \alpha \) and \( \beta \) we get,

\[
\frac{|A|^2}{|E|^2} = T^{-1} = \frac{1}{4} \left[ \left( 1 + \frac{\sqrt{2m(E-W_0)}}{\sqrt{2mE}} \right)^2 + \sinh^2 \left( \frac{L}{\hbar} \sqrt{2m(V_0 - E)} \right) \right] \left[ \left( 1 + \frac{\sqrt{2m(E-W_0)}}{\sqrt{2mE}} \right)^2 + \frac{\sqrt{2m(V_0 - E)}}{\sqrt{2mE}} \right] \left[ \left( 1 + \frac{\sqrt{2m(E-W_0)}}{\sqrt{2mE}} \right)^2 - \frac{\sqrt{2m(V_0 - E)}}{\sqrt{2mE}} \right] \left[ \left( 1 + \frac{\sqrt{2m(E-W_0)}}{\sqrt{2mE}} \right)^2 \right]
\]

\[
= \frac{1}{4} \left[ \left( 1 + \frac{\sqrt{E-W_0}}{E} \right)^2 + \sinh^2 \left( \frac{L}{\hbar} \sqrt{2m(V_0 - E)} \right) \right] \left[ \left( 1 + \frac{\sqrt{E-W_0}}{E} \right)^2 + \frac{\sqrt{V_0 - E}}{\sqrt{V_0 - E}} \right] \left[ \left( 1 + \frac{\sqrt{E-W_0}}{E} \right)^2 \right].
\]
(g) If the barrier in figure (a) is to act like a 50:50 beamsplitter, what are the required conditions on $E$, $V_0$ and $L$?

**Answer (g):**

If the barrier acts like a 50:50 beamsplitter, the transmission probability will be 0.5. Setting $T = 0.5$, in the last expression of part (e),

\[
\left[ 1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2 \left( \frac{L}{\hbar} \sqrt{2m(V_0 - E)} \right) \right]^{-1} = \frac{1}{2}
\]

\[1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2 \left( \frac{L}{\hbar} \sqrt{2m(V_0 - E)} \right) = 2\]

\[\frac{V_0^2}{4E(V_0 - E)} \sinh^2 \left( \frac{L}{\hbar} \sqrt{2m(V_0 - E)} \right) = 1\]

\[
\frac{4E(V_0 - E)}{V_0^2} = \sinh^2 \left( \frac{L}{\hbar} \sqrt{2m(V_0 - E)} \right)
\]

\[
\frac{\sqrt{4E(V_0 - E)}}{V_0} = \sinh \left( \frac{L}{\hbar} \sqrt{2m(V_0 - E)} \right)
\]

\[
\frac{2\sqrt{E\varepsilon}}{V_0} = \sinh \left( \frac{L}{\hbar} \sqrt{2m\varepsilon} \right),
\]

where $\varepsilon = V_0 - E$. The above expression is the required relation between $E$, $V_0$ and $L$. 