PHYS 4301
Homework 7

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1. You will explore some general properties of the so-called transfer matrix (1) for 1D scattering by potential feature $V(x)$ such that on its left $(x \to -\infty)$ and right $(x \to \infty)$ sides the potential is constant, examples being a potential step, a barrier, or a well. In the piecewise solution of the stationary Schrödinger equation (2), we relate the solution in the left part (3) to the solution in the right part (4) with the transfer matrix (5). Here energies are such that k_1 and k_2 are real (positive) quantities.

$$M = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \tag{1}$$

$$\hat{H}\psi = E\psi \tag{2}$$

$$\psi_1 = Aexp\left(ik_1x\right) + Bexp\left(-ik_1x\right) \tag{3}$$

$$\psi_2 = Cexp\left(ik_2x\right) + Dexp\left(-ik_2x\right) \tag{4}$$

$$\begin{pmatrix} C \\ D \end{pmatrix} = M \begin{pmatrix} A \\ B \end{pmatrix} \tag{5}$$

a) It is evident that if Eq. (2) holds for ψ, it also holds for ψ^* such that $\hat{H}\psi^* = E\psi^*$. Use this fact with functions (3) and (4) to establish that elements of matrix M in (1) actually satisfy the following restrictions:

$$d = a^* \tag{6}$$

$$c = b^* \tag{7}$$

$$\begin{aligned}
\begin{pmatrix} C \\ D \end{pmatrix} &= M \begin{pmatrix} A \\ B \end{pmatrix} \\
&= \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} \\
&= \begin{pmatrix} Aa + Bb \\ Ac + Bd \end{pmatrix} \\
C &= Aa + Bb \\
D &= Ac + Bd
\end{aligned}$$

Given that the potential $V(x)$ is real, we know that $V(x) = V^*(x)$. So, for the solution of the Schrödinger equation for $V^*(x)$, we know that the following are solutions:

$$\psi_1^*(x) = B^* e^{ik_1 x} + A^* e^{-ik_1 x}$$
$$\psi_2^*(x) = D^* e^{ik_2 x} + C^* e^{-ik_2 x}$$

Because these are solutions, their coefficients can be plugged into the transfer matrix equation (similar to ψ_1 and ψ_2):

$$\begin{aligned} \begin{pmatrix} C^* \\ D^* \end{pmatrix} &= M \begin{pmatrix} A^* \\ B^* \end{pmatrix} \\ &= \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} A^* \\ B^* \end{pmatrix} \end{aligned}$$

Taking the complex conjugate of both sides of this equation, we get:

$$\begin{pmatrix} C \\ D \end{pmatrix} = \begin{pmatrix} a^* & b^* \\ c^* & d^* \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix}$$

We can rewrite this by swapping rows and columns, retaining the identity:

$$\begin{pmatrix} D \\ C \end{pmatrix} = \begin{pmatrix} d^* & c^* \\ b^* & a^* \end{pmatrix} \begin{pmatrix} B \\ A \end{pmatrix}$$

Because we've retained the identity, we can set the transfer matrix equal to our modified transfer matrix:

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} d^* & c^* \\ b^* & a^* \end{pmatrix}$$

And therefore, $\boxed{d = a^*}$ and $\boxed{c = b^*}$.

b) Calculate the transfer matrix for the 1D delta-function potential feature (8) where γ characterizes its sign and strength. Verify that the resulting matrix obeys general relationships (6) and (7).

$$V(x) = \frac{\hbar^2}{m}\gamma\delta(x) \tag{8}$$

For $x < 0$, $V = 0$:

$$\psi_1(x) = Ae^{ikx} + Be^{-ikx}$$

For $x > 0$, $V = 0$:

$$\psi_2(x) = Ce^{ikx} + De^{-ikx}$$

When $x = 0$, $\psi_1(x) = \psi_2(x) \to A + B = C + D$. Plugging this identity into the Schrödinger equation, we get:

$$\begin{aligned}
0 &= \left(\psi_2'(0) - \psi_1'(0)\right) - 2\gamma\psi_1(0) \\
0 &= ik\left((C-D) - (A-B)\right) - 2\gamma(A+B) \\
C - D &= \left(1 + \frac{2\gamma}{ik}\right)A - \left(1 - \frac{2\gamma}{ik}\right)B \\
&= \left(1 - \frac{2\gamma i}{k}\right)A - \left(1 + \frac{2\gamma i}{k}\right)B \\
(C+D) + (C-D) = 2C &= \left(2 - \frac{2\gamma i}{k}\right)A - \left(\frac{2\gamma i}{k}\right)B \\
(C+D) - (C-D) = 2D &= \left(\frac{2\gamma i}{k}\right)A + \left(2 + \frac{2\gamma i}{k}\right)B \\
\begin{pmatrix} C \\ D \end{pmatrix} &= \begin{pmatrix} 1 - \frac{\gamma i}{k} & -\frac{\gamma i}{k} \\ \frac{\gamma i}{k} & 1 + \frac{\gamma i}{k} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} \\
M &= \boxed{\begin{pmatrix} 1 - \frac{\gamma i}{k} & -\frac{\gamma i}{k} \\ \frac{\gamma i}{k} & 1 + \frac{\gamma i}{k} \end{pmatrix}}
\end{aligned}$$

c) Use now the fact that the probability current density is the same on the left and the right sides of $V(x)$ to establish another general relation that determinant of the transfer matrix:

$$det(M) = |a|^2 - |b|^2 = \frac{k_1}{k_2}. \tag{9}$$

$$\begin{aligned} det(M) &= \begin{vmatrix} 1 - \frac{\gamma i}{k} & -\frac{\gamma i}{k} \\ \frac{\gamma i}{k} & 1 + \frac{\gamma i}{k} \end{vmatrix} \\ &= \frac{(k - i\gamma)(k + i\gamma)}{k^2} - \frac{\gamma^2}{k^2} \\ &= \frac{k^2 + \gamma^2}{k^2} - \frac{\gamma^2}{k^2} \\ &= \frac{k^2}{k^2} = 1 \end{aligned}$$

Therefore the probability density must be the same on the left and right sides, so (9) must be true.

d) In terms of the elements of transfer matrix (1), find the reflection R and transmission T coefficients for the particles incident from the left and for particles incident from the right. Use general relations established above to prove that the reflection coefficients for particles incident from the left and for particles incident from the right are exactly the same independently of the shape of the potential feature $V(x)$ "in the middle" (the difference can be only in phase factors).

The transfer matrix can be expressed in the form:

$$\begin{pmatrix} t' - \frac{rr'}{t} & \frac{r}{t} \\ -\frac{r'}{t} & \frac{1}{t} \end{pmatrix}$$

where $T = |t|^2$ and $R = |r|^2$. This gives us the equations:

$$\begin{aligned} a &= t' - rt^{-1}r' \\ b &= rt^{-1} \\ c &= -t^{-1}r' \\ d &= t^{-1} \end{aligned}$$

Therefore,

$$\begin{aligned} t &= \frac{1}{d} \\ r &= bt = \frac{b}{d} \end{aligned}$$

So, $T = \boxed{\left|\frac{1}{d}\right|^2}$, $R = \boxed{\left|\frac{b}{d}\right|^2}$

2. We are interested in the transmission coefficient T for the particles of energy E incident "from the left" $(x \to -\infty)$ on the square potential feature (10), where V_0 and a are the respective energy and length parameters ($V_0 > 0$ describes a potential barrier and $V_0 < 0$ a potential well). As usual, it is convenient to relate energy E to the wave-numbers in the corresponding regions of space (11), assuming for now that $E > V_0$. The setup of our problem (incident from the left) implies that region $x > a$ features only a transmitted wave.

$$V(x) = \begin{cases} 0, & |x| > a \\ V_0, & |x| < a \end{cases} \tag{10}$$

$$\frac{\hbar^2 k_1^2}{2m} = E, \quad \frac{\hbar^2 k_2^2}{2m} = E - V_0 \tag{11}$$

a) Write down the wave function continuity equations at regional boundaries $x = -a$ and $x = a$.

For $x \leq -a$,

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0$$
$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0$$
$$k_1^2 = \frac{2mE}{\hbar^2} \to \left(\frac{d^2}{dx^2} + k_1^2\right)\psi = 0$$
$$\frac{d^2}{dx^2} = \pm ik_1$$
$$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}$$

For $-a < x < a$,

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\psi = 0$$
$$k_2^2 = \frac{2m}{\hbar^2}(E - V_0)$$
$$\left(\frac{d^2}{dx^2} + k_1^2\right)\psi = 0$$
$$\frac{d^2}{dx^2} = \pm ik_2$$
$$\psi_2(x) = Ce^{ik_2x} + De^{-ik_2x}$$

For $x \geq a$,

$$\psi_3(x) = Ee^{ik_1x}$$

Boundary conditions:

$$\psi_1(-a) = \psi_2(-a) + \psi_2^{'}(-a) = \psi_2^{'}(-a)$$
$$\psi_2(a) = \psi_3(a) + \psi_2^{'}(a) = \psi_3^{'}(a)$$

b) Solve those equations for appropriate variables to derive the transmission coefficient (12). Does equation (12) describe transmission resonances with $T = 1$? At what energies E?

$$T = \left[1 + \frac{1}{4}\left(\frac{k_1}{k_2}\right)^2 sin^2\left(2k_2 a\right)\right]^{-1} \tag{12}$$

$$\begin{aligned}
\psi_1\left(-a\right) &= \psi_2\left(-a\right) \\
Ae^{-ik_1 a} + Be^{ik_1 a} &= Ce^{-ik_2 a} + De^{ik_2 a} \\
\psi_1^{'}\left(-a\right) &= \psi_2^{'}\left(-a\right) \\
k_1\left[Ae^{-ik_1 a} + Be^{ik_1 a}\right] &= k_2\left[Ce^{-ik_2 a} - De^{ik_2 a}\right]
\end{aligned}$$

$$\begin{aligned}
\psi_2\left(a\right) &= \psi_3\left(a\right) \\
Ce^{-ik_2 a} + De^{-ik_2 a} &= Ee^{-ik_1 a} \\
\psi_2^{'}\left(a\right) &= \psi_3^{'}\left(a\right) \\
k_2\left[Ce^{-ik_2 a} - De^{-ik_2 a}\right] &= k_1 Ee^{-ik_1 a} \\
2Ak_1\left(e^{-ik_1 a}\right) &= Ce^{-ik_2 a}\left(k_1 + k_2\right) + De^{ik_2 a}\left(k_1 - k_2\right) \\
2e^{ik_2 a}Cik_2 &= iE\left(k_2 + k_1\right)e^{ik_1 a} \\
C &= \frac{E}{2k_2}\left(k_2 + k_1\right)e^{i(k_1 - k_2)a} \\
2Dik_2 e^{-ik_2 a} &= iE\left(k_2 - k_1\right)e^{ik_1 a} \\
D &= \frac{E}{2k_2}\left(k_2 - k_1\right)e^{i(k_1 + k_2)a}
\end{aligned}$$

$$\begin{aligned}
2Ak_1 e^{-ik_1 a} &= \frac{E}{2k_2}\left(k_1 + k_2\right)^2 e^{ik_1 a - ik_2 a - ik_2 a} - \frac{E}{2k_2}\left(k_2 - k_1\right)^2 e^{ik_1 a + ik_2 a + ik_2 a} \\
2Ak_1 e^{-ik_1 a} &= \frac{E}{2k_2}e^{ik_1 a}\left[\left(k_1 + k_2\right)^2 e^{-2ik_2 a} - \left(k_2 - k_1\right)^2 e^{2ik_2 a}\right] \\
\frac{4k_1 k_2 e^{-2ik_1 a}A}{E} &= \left[\left(k_1^2 + k_2^2 + 2k_1 k_2\right)e^{-2ik_2 a} - \left(k_1^2 + k_2^2 - 2k_1 k_2\right)e^{2ik_2 a}\right] \\
&= \left[-\left(k_1^2 + k_2\right)\left(e^{2ik_2 a} - e^{-2ik_2 a}\right) + 2k_1 k_2\left(e^{2ik_2 a} + e^{-2ik_2 a}\right)\right] \\
&= 4k_1 k_2 cos\left(2k_2 a\right) - 2i\left(k_1^2 + k_2^2\right) sin\left(2k_2 a\right)
\end{aligned}$$

$$\begin{aligned}
T = \left|\frac{E}{A}\right|^2 &= \frac{16k_1^2 k_2^2\left|e^{-2ik_1 a}\right|^2}{\left(4k_1 k_2\right)^2 cos^2\left(2k_2 a\right) + 4\left(k_1^2 + k_2^2\right)^2 sin^2\left(2k_2 a\right)} \\
&= \frac{16k_1^2 k_2^2}{\left(4k_1 k_2\right)^2\left(1 - sin^2\left(2k_2 a\right)\right) + 4\left(k_1^2 + k_2^2\right)^2 sin^2\left(2k_2 a\right)} \\
&= \frac{1}{1 + \frac{1}{4k_1^2 k_2^2}\left(k_1^4 + k_2^4 - 2k_1^2 k_2^2\right) sin^2\left(2k_2 a\right)} \\
&= \boxed{\left[1 + \frac{1}{4}\left(\frac{k_1}{k_2} - \frac{k_2}{k_1}\right)^2 sin^2\left(2k_2 a\right)\right]^{-1}}
\end{aligned}$$

c) The solution developed can also be used for under-the-barrier transmission with $E < V_0$ by exploiting a formal substitution $k_2 = i\kappa_2$ where we now have (13) instead of (9). Write down the corresponding modified expression for T in terms of k_1 and κ_2. Does that expression describe transmission resonances? Is it supposed to?

$$\frac{\hbar^2\kappa_2^2}{2m} = V_0 - E \tag{13}$$

For $E < V_0$,

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

d) Show that the under-the-barrier transmission derived in the previous item becomes exponentially small for sufficiently wide (or high) barriers:

$$T \simeq \frac{16E\left(V_0 - E\right)}{V_0^2} exp\left(-\frac{4a}{\hbar}\sqrt{2m\left(V_0 - E\right)}\right) \tag{14}$$

For high barriers, we can perform the following approximation:

$$sinh\left(\frac{2a}{\hbar}\sqrt{2m\left(V_0 - E\right)}\right) \simeq \frac{1}{2}e^{\frac{2a}{\hbar}\sqrt{2m(V_0-E)}}$$

Therefore,

$$\begin{aligned} T &\simeq \left[\frac{V_0^2}{4E\left(V_0 - E\right)}\left(\frac{1}{2}e^{\frac{2a}{\hbar}\sqrt{2m(V_0-E)}}\right)^2\right]^{-1} \\ &= \frac{16E\left(V_0 - E\right)}{V_0^2}e^{-\frac{4a}{\hbar}\sqrt{2m(V_0-E)}} \end{aligned}$$