Homework 8 - Piecewise Constant Potential, Delta Function Potential

Question 1:

Consider a step function potential $V(x) = V_0 \Theta(x)$ and particles with energy $E > V_0$ incident on it from both sides simultaneously. The wave function is

$$\psi(x) = \begin{cases} Ae^{ik_1 x} + Be^{-ik_1 x}, & x < 0, \\ Ce^{ik_2 x} + De^{-ik_2 x}, & x > 0, \end{cases}$$

where $k_1 = \sqrt{2mE}/\hbar$ and $k_2 = \sqrt{2m(E - V_0)}/\hbar$

1. Find the boundary conditions and write down the matching conditions for the coefficients.
2. Determine the matrix U defined by the relation
$$\begin{pmatrix} \sqrt{k_2}C \\ \sqrt{k_1}B \end{pmatrix} = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix} \begin{pmatrix} \sqrt{k_1}A \\ \sqrt{k_2}D \end{pmatrix},$$
and show that $UU^\dagger = U^\dagger U = I$ where I is the standard 2×2 unit matrix. This kind of matrix (operator) is called a unitary matrix (operator).
3. Write down the probability current conservation and show that it is directly related to the unitarity of the matrix U.

Solution:

1. The boundary conditions are
$$\psi(0_-) = \psi(0_+) \quad \text{and} \quad \psi'(0_-) = \psi'(0_+).$$
Plugging in the wave function we get
$$A + B = C + D \quad \text{and} \quad k_1(A - B) = k_2(C - D).$$
2. From the conditions above we get
$$2Ak_1 = C(k_1 + k_2) + D(k_1 - k_2) \quad \rightarrow \quad C = \frac{2k_1}{k_1 + k_2}A + \frac{k_2 - k_1}{k_1 + k_2}D,$$
$$A(k_2 - k_1) + B(k_1 + k_2) = 2k_2 D \quad \rightarrow \quad B = \frac{k_1 - k_2}{k_1 + k_2}A + \frac{2k_2}{k_1 + k_2}D.$$
Therefore
$$\boxed{\begin{pmatrix} \sqrt{k_2}C \\ \sqrt{k_1}B \end{pmatrix} = \frac{1}{k_1 + k_2} \begin{pmatrix} 2\sqrt{k_1 k_2} & k_2 - k_1 \\ k_1 - k_2 & 2\sqrt{k_1 k_2} \end{pmatrix} \begin{pmatrix} \sqrt{k_1}A \\ \sqrt{k_2}D \end{pmatrix}}.$$
We want to show that $U^\dagger = U^{-1}$, since k_1 and k_2 are real, then $\overline{U} = U$, thus
$$U^\dagger = \left(\overline{U}\right)^T = U^T = \frac{1}{k_1 + k_2} \begin{pmatrix} 2\sqrt{k_1 k_2} & k_1 - k_2 \\ k_2 - k_1 & 2\sqrt{k_1 k_2} \end{pmatrix},$$
whereas
$$U^{-1} = \frac{1}{\underbrace{\det U}_{=1}} \text{adj} U = \frac{1}{k_1 + k_2} \begin{pmatrix} 2\sqrt{k_1 k_2} & k_1 - k_2 \\ k_2 - k_1 & 2\sqrt{k_1 k_2} \end{pmatrix} = U^T.$$
thus
$$\boxed{UU^\dagger = U^\dagger U = I_{2\times 2}}.$$

3. Probability current conservation means $J_i^- + J_r^- = J_i^+ + J_r^+$, in our case

$$J_i^- = \frac{\hbar}{m}\text{Im}\left[\psi_{i-}^*\frac{\partial\psi_{i-}}{\partial x}\right] = \frac{\hbar k_1}{m}|A|^2, \qquad J_r^- = \frac{\hbar}{m}\text{Im}\left[\psi_{r-}^*\frac{\partial\psi_{r-}}{\partial x}\right] = -\frac{\hbar k_1}{m}|B|^2,$$
$$J_i^+ = \frac{\hbar}{m}\text{Im}\left[\psi_{i+}^*\frac{\partial\psi_{i+}}{\partial x}\right] = \frac{\hbar k_2}{m}|C|^2, \qquad J_r^+ = \frac{\hbar}{m}\text{Im}\left[\psi_{r+}^*\frac{\partial\psi_{r+}}{\partial x}\right] = -\frac{\hbar k_2}{m}|D|^2,$$

which yield

$$k_1\left(|A|^2 - |B|^2\right) = k_2\left(|C|^2 - |D|^2\right) \quad \to \quad k_2|C|^2 + k_1|B|^2 = k_1|A|^2 + k_2|D|^2.$$

Using the matrix notation we can write the right-hand-side as

$$\begin{aligned} k_2|C|^2 + k_1|B|^2 &= \begin{pmatrix} \sqrt{k_2}C^* & \sqrt{k_1}B^* \end{pmatrix}\begin{pmatrix} \sqrt{k_2}C \\ \sqrt{k_1}B \end{pmatrix} \\ &= \left[U\begin{pmatrix} \sqrt{k_1}A \\ \sqrt{k_2}D \end{pmatrix}\right]^\dagger U\begin{pmatrix} \sqrt{k_1}A \\ \sqrt{k_2}D \end{pmatrix} \\ &= \begin{pmatrix} \sqrt{k_1}A^* & \sqrt{k_2}D^* \end{pmatrix} U^\dagger U\begin{pmatrix} \sqrt{k_1}A \\ \sqrt{k_2}D \end{pmatrix} \\ &= k_1|A|^2 + k_2|D|^2, \end{aligned}$$

so that the unitarity of U implies the conservation of the probability current and vice versa.

Question 2:

Consider a one dimensional infinite square well with a very short range force in its centre, represented by a delta function potential. The potential energy s given by

$$V(x) = \begin{cases} \infty, & x < -L, \\ \frac{\hbar^2 g}{2m}\delta(x), & -L < x < L, \\ \infty, & x > L. \end{cases}$$

First, consider $g < 0$. This represents an attractive force at the centre of the well.

1. For $E > 0$, find the energy eigenvalues of the system.
2. Are there any bound states in the case of $E < 0$?

   Now, change to a repulsive force in the centre $g > 0$.

3. What is the energy spectrum for the system now?
4. For the limit $g \to \infty$, find energy eigenvalues exactly.

Solution:

1. Note that we can expect *odd* and *even* solutions, since the potential is symmetric. However, let us not assume that in advance, and see the this property emerges naturally. For $E > 0$, the solution inside the well is that of a free particle, thus

$$\psi(x) = \begin{cases} 0, & x \le -L, \\ Ae^{ikx} + Be^{-ikx}, & -L < x < 0, \\ Ce^{ikx} + De^{-ikx}, & 0 < x < L, \\ 0, & x \ge L, \end{cases} \qquad \text{where } k \equiv \frac{\sqrt{2mE}}{\hbar}.$$

   The boundary conditions are

$$\psi(0_+) = \psi(0_-): \quad C + D = A + B \tag{1}$$
$$\psi(-L) = 0: \quad Ae^{-ikL} + Be^{ikL} = 0 \tag{2}$$
$$\psi(L) = 0: \quad Ce^{ikL} + De^{-ikL} = 0 \tag{3}$$
$$\psi'(0_+) - \psi'(0_-) = g\psi(0): \quad ik(C - D - A + B) = g(A + B) \tag{4}$$

Plugging (2) and (3) into (1) we find

$$D\left(1-e^{-2ikL}\right)=A\left(1-e^{-2ikL}\right)\quad\rightarrow\quad D=A,\quad\text{or}\quad k_n=\frac{\pi n}{L},$$

where the second option corresponds to a set of allowed energies

$$\boxed{E_n=\frac{\pi^2\hbar^2n^2}{2mL^2}},$$

which are just the allowed energies in an infinite square well, and they corresponds to the *odd* eigenstates, since it follows that $A=-B$ and $C=-D$, which result in a sine function.
The other solution is for $D=A$: using (1) plus (2) now yield

$$C=B=-Ae^{-2ikL},$$

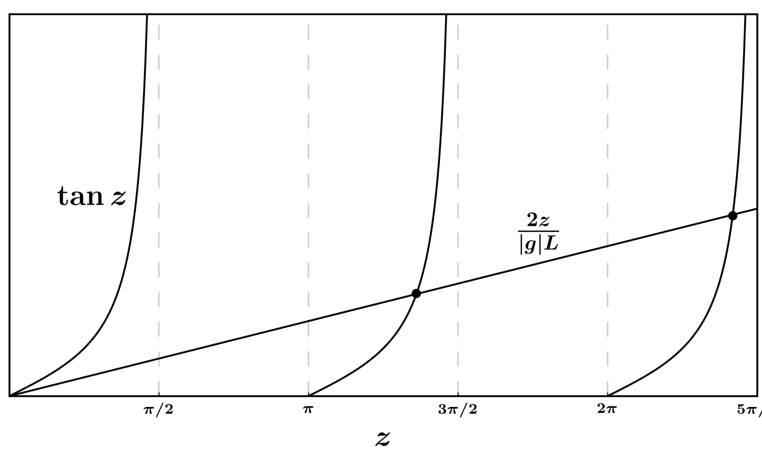
it is easy to see, by plugging it into our general solution, that it corresponds to even *eigenstates.* Plugging the three relations into (4) gives us

$$-2ik\left(1+e^{-2ikL}\right)=g\left(1-e^{-2ikL}\right)\quad\rightarrow\quad\frac{2z}{gL}=-\tan z,\qquad\text{where } z\equiv kL.$$

In the case of $g<0$ this reads

$$\boxed{\frac{2z}{|g|\,L}=\tan z},$$

and the allowed energies are determined from the crossing points of the curves of two functions of k in both sides of the equation. Note that for $g\rightarrow 0$ this equation has no solution and we are left with the allowed energies of an infinite square well, as expected.



2. For $E<0$, the solution inside the well is that of a free particle, thus

$$\psi(x)=\begin{cases}0, & x\leq -L,\\ Ae^{\kappa x}+Be^{-\kappa x}, & -L<x<0,\\ Ce^{\kappa x}+De^{-\kappa x}, & 0<x<L,\\ 0, & x\geq L,\end{cases}\qquad\text{where } \kappa\equiv\frac{\sqrt{-2mE}}{\hbar}$$

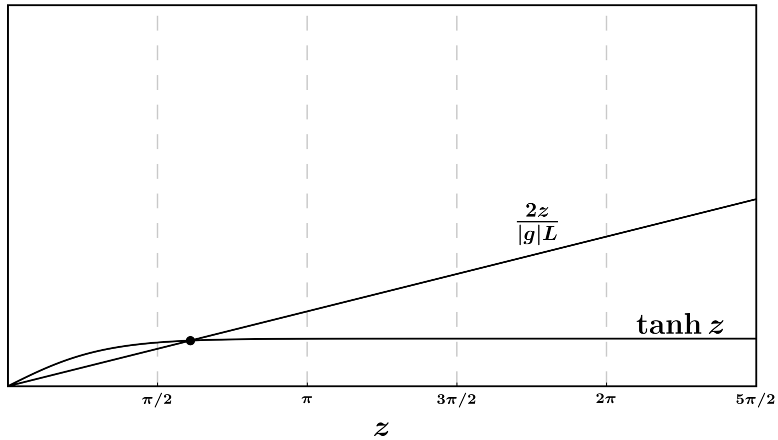
Basically, the results are the same, only with $ik\rightarrow\kappa$, thus

$$-2\kappa\left(e^{-2\kappa L}+1\right)=g\left(1-e^{-2\kappa L}\right)\quad\rightarrow\frac{2z}{gL}=-\tanh z,\qquad\text{where } z\equiv\kappa L.$$

In the case of $g<0$ this reads

$$\boxed{\frac{2z}{|g|\,L}=\tanh z},$$

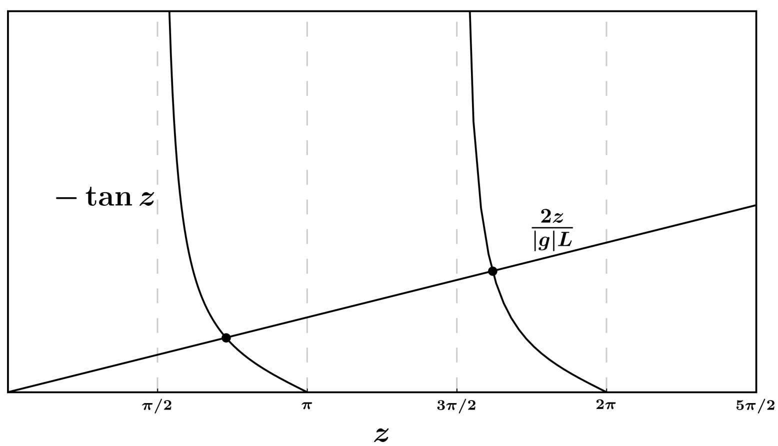
and the allowed energies are determined from the crossing points of the curves of two functions of κ in both sides of the equation: in this case there is only a single allowed stat, only if $|g| > \frac{2}{L}$.



3. For $g > 0$ we get

$$E > 0: \quad \frac{2z}{gL} = -\tan z, \qquad \text{where } z \equiv kL \text{ and } k \equiv \frac{\sqrt{2mE}}{\hbar},$$
$$E < 0: \quad \frac{2z}{gL} = -\tanh z, \qquad \text{where } z \equiv \kappa L \text{ and } \kappa \equiv \frac{\sqrt{-2mE}}{\hbar}.$$

While the $E > 0$ case yields bounded states, in the $E < 0$ case there are no allowed energies since $\tanh z \geq 0$ for $z > 0$, which is also anticipated since $E < \min[V(x)]$ hence there are no physical solutions.



4. For $g \to \infty$ the left-hand-side in the equation for the energy goes to zero, in which case, the equation reads

$$\tan kL = 0 \quad \text{or} \quad k_n = \frac{n\pi}{L} \quad \to \quad \boxed{E_n = \frac{\pi^2\hbar^2 n^2}{2mL^2}},$$

which are, again, the allowed energies for the infinite square well. It can be thought of as if $g \to \infty$ corresponds to two adjacent infinite wells, so that each contributes energy E_n to the total system and together they form the complete set of eigenstates of the system.

Question 3:

Consider a finite square potential barrier

$$V(x) = \begin{cases} 0, & x < -L, \\ V_0, & -L < x < L, \\ 0, & x > L, \end{cases}$$

and particles incident to it on both sides simultaneously. The solution of Schrödinger equation in the regions outside the barrier yield

$$\psi = \begin{cases} Ae^{ikx} + Be^{-ikx}, & x < -L, \\ Ce^{ikx} + De^{-ikx}, & x > L, \end{cases}$$

where $k = \sqrt{2mE}/\hbar$. Using the system's boundary conditions we can get a relation of the sort

$$\begin{pmatrix} C \\ B \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} A \\ D \end{pmatrix}$$

1. Find matrix elements M_{ij} for the two cases $E > V_0$ and $V_0 > E > 0$.
2. Show that the matrix M is also unitary.
3. Calculate the probability current on both sides of the barrier and show that it is conserved for both cases.
4. Calculate transmission and reflection coefficients for both cases.
5. Repeat the calculation for a potential well

$$V(x) = \begin{cases} 0, & x < -L, \\ -V_0, & -L < x < L, \\ 0, & x > L, \end{cases}$$

given that $E > 0$.

Solution:

1. Inside the barrier the general solution is

$$\psi(x) = Fe^{ik'x} + Ge^{-ik'x}, \quad -L < x < L,$$

where $k' \equiv \sqrt{2m(E - V_0)}/\hbar$ is imaginary or real, depends on the sign of $(E - V_0)$. Using the boundary conditions we have

$$\begin{aligned} \psi(-L_-) = \psi(-L_+): &\quad Ae^{-ikL} + Be^{ikL} = Fe^{-ik'L} + Ge^{ik'L} \\ \psi'(-L_-) = \psi'(-L_+): &\quad k\left(Ae^{-ikL} - Be^{ikL}\right) = k'\left(Fe^{ik'L} - Ge^{-ik'L}\right) \\ \psi(L_-) = \psi(L_+): &\quad Fe^{ik'L} + Ge^{-ik'L} = Ce^{ikL} + De^{-ikL} \\ \psi'(L_-) = \psi'(L_+): &\quad k'\left(Fe^{ik'L} - Ge^{-ik'L}\right) = k\left(Ce^{ikL} - De^{-ikL}\right). \end{aligned}$$

Eliminating F and G, we may find the expressions for C and B in terms of D and A:

$$C = \frac{De^{-2ikL}\left(k^2 - k'^2\right)\left(-1 + e^{4ik'L}\right) - 4Akk'e^{-2i(k-k')L}}{-\left(k + k'\right)^2 + \left(k - k'\right)^2 e^{4ik'L}},$$

$$B = \frac{Ae^{-2ikL}\left(k^2 - k'^2\right)\left(-1 + e^{4ik'L}\right) - 4Dkk'e^{-2i(k-k')L}}{-\left(k + k'\right)^2 + \left(k - k'\right)^2 e^{4ik'L}},$$

hence

$$\boxed{\begin{pmatrix} C \\ B \end{pmatrix} = \frac{e^{-2ikL}}{-\left(k + k'\right)^2 + \left(k - k'\right)^2 e^{4ik'L}} \begin{pmatrix} -4kk'e^{2ik'L} & \left(k^2 - k'^2\right)\left(-1 + e^{4ik'L}\right) \\ \left(k^2 - k'^2\right)\left(-1 + e^{4ik'L}\right) & -4kk'e^{2ik'L} \end{pmatrix} \begin{pmatrix} A \\ D \end{pmatrix}},$$

where we have $\boxed{k' = \sqrt{2m(E - V_0)}/\hbar}$ if $E > V_0$ and $\boxed{k' = i\kappa = i\sqrt{2m(V_0 - E)}/\hbar}$ if $E < V_0$, with both k and κ as real parameters.

2. One can show that
$$\boxed{M^\dagger M = I_{2\times 2}}.$$

3. The probability current on each side reads
$$\begin{aligned}
J_L &= \frac{\hbar}{m}\mathrm{Im}\left[\left(Ae^{ikx}+Be^{-ikx}\right)^* ik\left(Ae^{ikx}-Be^{-ikx}\right)\right] \\
&= \frac{\hbar}{m}\mathrm{Im}\left[ik\left(|A|^2+\underbrace{AB^*e^{2ikx}-A^*Be^{-2ikx}}_{\text{real}}-|B|^2\right)\right],
\end{aligned}$$
hence
$$\boxed{J_L = \frac{\hbar k}{m}\left(|A|^2-|B|^2\right)},$$
similarly
$$\boxed{J_R = \frac{\hbar k}{m}\left(|C|^2-|D|^2\right)}.$$
Conservation of the current means
$$J_L = J_R \quad \to \quad |A|^2+|D|^2 = |C|^2+|B|^2\,.$$
The left-hand-side can be written as
$$|A|^2+|D|^2 = \begin{pmatrix} A^* & D^* \end{pmatrix}\begin{pmatrix} A \\ D \end{pmatrix} = \begin{pmatrix} C^* & B^* \end{pmatrix}\underbrace{M^\dagger M}_{I_{2\times 2}}\begin{pmatrix} C \\ B \end{pmatrix} = \begin{pmatrix} C^* & B^* \end{pmatrix}\begin{pmatrix} C \\ B \end{pmatrix} = |C|^2+|B|^2\,,$$
which means $\boxed{J_L = J_R}$.

4. The transmission and reflection coefficients are, due to symmetry, the same to each direction, thus let us consider the ones for a particle incidents from the left:
$$\begin{aligned}
T_L &= \frac{J_R^+}{J_L^+} = \frac{|C|^2}{|A|^2} = |M_{11}|^2 = \frac{16k^2\,|k'|^2}{\left|-\left(k+k'\right)^2e^{-2ik'L}+\left(k-k'\right)^2e^{2ik'L}\right|^2}, \\
R_L &= 1-T_L.
\end{aligned}$$
For $E > V_0$ we have
$$\begin{aligned}
T_L &= \frac{\left(4kk'\right)^2}{\left|\left(k+k'\right)^2e^{-2ik'L}-\left(k-k'\right)^2e^{2ik'L}\right|^2} \\
&= \frac{\left(4kk'\right)^2}{\left[\left(k+k'\right)^2-\left(k-k'\right)^2\right]^2\cos^2 k'L+\left[\left(k+k'\right)^2+\left(k-k'\right)^2\right]^2\sin^2 2k'L},
\end{aligned}$$
$$\boxed{T_L = \frac{4k^2k'^2}{4k^2k'^2\cos^2 k'L+\left(k^2+k'^2\right)^2\sin^2 2k'L}}.$$
For $E < V_0$ we have
$$\begin{aligned}
T_L &= \frac{\left(4k\kappa\right)^2}{\left|\left(k+i\kappa\right)^2e^{2\kappa L}-\left(k-i\kappa\right)^2e^{-2\kappa L}\right|^2} \\
&= \frac{\left(4k\kappa\right)^2}{\left|\left(k^2+2ik\kappa-\kappa^2\right)e^{2\kappa L}-\left(k^2-2ik\kappa-\kappa^2\right)e^{-2\kappa L}\right|^2} \\
&= \frac{\left(4k\kappa\right)^2}{\left|2\left(k^2-\kappa^2\right)\sinh 2\kappa L+4ik\kappa\cosh 2\kappa L\right|^2},
\end{aligned}$$
$$\boxed{T_L = \frac{4k^2\kappa^2}{4k^2\kappa^2\cosh^2 2\kappa L+\left(k^2-\kappa^2\right)^2\sinh^2 2\kappa L}}.$$

5. Since we solved for a general k and k' we can use this solution for $V_0 \to -V_0$. For this potential there is only solution if $E \geq -V_0$, in which case, the solutions are the same as the ones for $E > 0$ with a real $k' \equiv \sqrt{2m(E+V_0)}/\hbar$, inside the barrier, and real $k \equiv \sqrt{2mE}$ if $E > 0$ or imaginary $k \equiv i\kappa = \sqrt{-2mE}$ is $E < 0$.

Question 4:

Consider an incidence of particles with $E > 0$ moving in a potential consisting of two unequal delta functions

$$V(x) = \frac{\hbar^2}{2m}\left[g_1\delta(x+a) + g_2\delta(x-a)\right].$$

1. Calculate the transmission coefficient.
2. Consider the case $g_1 = -g_2$ and show that for some values of energy we get perfect transmission and no reflection. Explain this result, give a qualitative argument as to why wave functions with these energies don't notice the potential.

Solution:

1. The solution is that of a free particle

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & x < -a, \\ Fe^{ikx} + Ge^{-ikx}, & -a < x < a, \\ Ce^{ikx}, & x > a, \end{cases} \qquad \text{with } k \equiv \frac{\sqrt{2mE}}{\hbar},$$

where we assumed the particle propagates from the left. The boundary conditions are

$$\begin{aligned} \psi(-a_-) = \psi(-a_+): &\quad Ae^{-ika} + Be^{ika} = Fe^{-ika} + Ge^{ika} \\ \psi'(-a_+) - \psi'(-a_-) = g_1\psi(-a): &\quad ik\left(Fe^{ika} - Ge^{-ika} - Ae^{-ika} + Be^{ika}\right) = g_1\left(Ae^{-ika} + Be^{ika}\right) \\ \psi(L_-) = \psi(L_+): &\quad Fe^{ika} + Ge^{-ika} = Ce^{ika} \\ \psi'(L_-) = \psi'(L_+): &\quad ik\left(Ce^{ika} - Fe^{ikL} + Ge^{-ikL}\right) = g_2Ce^{ika}. \end{aligned}$$

Solving for B, F, G and C we get

$$C = \frac{4k^2}{g_1g_2e^{4iak} + (2k+ig_1)(2k+ig_2)}A$$

$$\boxed{T = \frac{J_t}{J_i} = \frac{|C|^2}{|A|^2} = \left[\left(1 + \frac{g_1g_2}{4k^2}(\cos 4ak - 1)\right)^2 + \left(\frac{g_1+g_2}{2k} + \frac{g_1g_2}{4k^2}\sin 4ak\right)^2\right]^{-1}}.$$

2. In the case of $g_1 = -g_2 \equiv g$ we find

$$T = \left[\left(1 - \frac{g^2}{4k^2}(\cos 4ak - 1)\right)^2 + \left(\frac{g^2}{4k^2}\sin 4ak\right)^2\right]^{-1}.$$

It is easy to see that we get $T = 1$ if $k_n = \frac{\pi n}{2a}$, which translates to

$$\boxed{E_n = \frac{\pi^2 h^2 n^2}{8ma^2}}.$$

The reason that such energies correspond to full transmission is that the wavelength is a multiple of the distance between the barriers.