Tutorial 9 - Delta Function Potential, Finite Potential well

Question 1:

Consider particles with energy $E > 0$ that are scattered of a delta function potential $V(x) = g\delta(x)$ in 1D. Without loss of generality, assume particles incident from the left.

1. Define the boundary conditions for the system.
2. Find eigenfunctions. Write the solutions in the form $\psi_E(x) = e^{ikx} + S(k)\, e^{ik|x|}$.
3. For $g < 0$, find a bound state $E < 0$. Find allowed energies. Show that this state corresponds to the pole of the function $S(k)$.

Solution:

The Schrödinger equation reads

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

1. We know that ψ must be continuous, otherwise ψ' would diverge somewhere hence the momentum and probability current would be infinite at this point, which is not physical. However, ψ' does not always have to be continuous, consider an integration of the Schrödinger equation over an infinitely small region around $x = 0$, namely $\epsilon < x < \epsilon$, and taking the limit of $\epsilon \to 0$:

$$-\frac{\hbar^2}{2m}\lim_{\epsilon\to 0}\underbrace{\int_{-\epsilon}^{\epsilon}\frac{d^2\psi}{dx^2}dx}_{\psi'\big|_{-\epsilon}^{\epsilon}} + g\lim_{\epsilon\to 0}\underbrace{\int_{-\epsilon}^{\epsilon}\delta(x)\,\psi(x)\,dx}_{=\psi(0)} = E\lim_{\epsilon\to 0}\int_{-\epsilon}^{\epsilon}\psi dx.$$

For sufficiently small ϵ the wave function on the right-hand-side can be treated as a constant, and integrating by parts the first term on the left, we find the boundary condition for ψ' to be

$$-\frac{\hbar^2}{2m}\lim_{\epsilon\to 0}\left[\psi'(\epsilon) - \psi'(-\epsilon)\right] + g\psi(0) = 2E\cancel{\lim_{\epsilon\to 0}\epsilon\psi} \quad\to\quad \Delta\psi' \equiv \psi'(0_+) - \psi'(0_-) = \frac{2mg}{\hbar^2}\psi(0).$$

Note that for a finite potential function $V(x)$ the potential term would vanish as well, leading to the condition of a continuous ψ' at $x = 0$.
Therefore, the boundary conditions at $x = 0$ are:

(a) $\psi(0_-) = \psi(0_+)$.
(b) $\psi'(0_+) - \psi'(0_-) = \alpha\psi(0)$, where $\alpha \equiv \frac{2mg}{\hbar^2}$.

2. Excluding the point $x = 0$, the Schrödinger equation reads

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \quad\to\quad \frac{d^2\psi}{dx^2} = -k^2\psi \quad \text{where } k \equiv \frac{\sqrt{2mE}}{\hbar} \quad \text{is real.}$$

The solution to this equation is of the form

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & x < 0, \\ Fe^{ikx} + Ge^{-ikx}, & x > 0. \end{cases}$$

Since we consider a particle that propagates from the left (i.e. from $x \to -\infty$ towards $x = 0$), which amplitude is represented by A, we have no reflection in the region $x > 0$, hence $G = 0$. The boundary conditions at $x = 0$ read

$$\psi(0_-) = \psi(0_+): \quad A + B = F,$$
$$\psi'(0_+) - \psi'(0_-) = \alpha\psi(0): \quad ik[F - (A - B)] = \alpha F,$$

$$(2ik - \alpha) B = \alpha A$$

which give us the relations

$$B = \frac{\alpha}{2ik - \alpha} A \quad \text{and} \quad F = \frac{2ik}{2ik - \alpha} A, \quad \text{where } \alpha \equiv \frac{2mg}{\hbar^2}.$$

Therefore, the solution is

$$\psi(x) = A \begin{cases} e^{ikx} + \frac{\alpha}{2ik-\alpha} e^{-ikx}, & x < 0, \\ \frac{2ik}{2ik-\alpha} e^{ikx}, & x > 0. \end{cases}$$

In order to write it in the form of $\psi_E(x) = e^{ikx} + S(k) e^{ik|x|}$ let us use the Heaviside function:

$$\begin{aligned}
\psi_E(x) &= A\Theta(-x)\left[e^{ikx} + \frac{\alpha}{2ik - \alpha} e^{-ikx}\right] + A\Theta(x)\left[\frac{2ik}{2ik - \alpha} e^{ikx}\right] \\
&= A\Theta(-x)\left[e^{ikx} + \frac{\alpha}{2ik - \alpha} e^{-ikx}\right] + A\Theta(x)\left[1 + \frac{\alpha}{2ik - \alpha}\right] e^{ikx} \\
&= Ae^{ikx}[\Theta(-x) + \Theta(x)] + A\frac{\alpha}{2ik - \alpha}\left[\Theta(-x) e^{-ikx} + \Theta(x) e^{ikx}\right] \\
&= A\left(e^{ikx} + \frac{\alpha}{2ik - \alpha} e^{ik|x|}\right),
\end{aligned}$$

thus

$$\boxed{\psi_E(x) = A\left(e^{ikx} + S(k) e^{ik|x|}\right), \quad \text{where } S(k) = \frac{\alpha}{2ik - \alpha}}.$$

3. For $E < 0$ the Schrödinger equation anywhere except $x = 0$ reads

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \quad \to \quad \frac{d^2\psi}{dx^2} = \kappa^2\psi, \text{ where } \kappa \equiv \frac{\sqrt{-2mE}}{\hbar} \quad \text{is real}$$

The solution to this equation is of the form

$$\psi(x) = \begin{cases} Ae^{\kappa x} + Be^{-\kappa x}, & x < 0, \\ Fe^{\kappa x} + Ge^{-\kappa x}, & x > 0. \end{cases}$$

We require $B = F = 0$ so that ψ will remain finite at $x \to \pm\infty$, while the boundary conditions read

$$\psi(0_-) = \psi(0_+): \quad A = G,$$
$$\psi'(0_+) - \psi'(0_-) = \alpha\psi(0): \quad -\kappa[G + A] = \alpha G,$$

that is

$$\kappa = -\frac{\alpha}{2} \quad \to \quad \frac{\sqrt{-2mE_0}}{\hbar} = \frac{m|g|}{\hbar^2} \quad \to \quad \boxed{E_0 = -\frac{m|g|^2}{2\hbar^2}},$$

thus, there is only one allowed energy, and the corresponding wave function is

$$\boxed{\psi(x) = Ae^{-\frac{m|g|}{\hbar^2}|x|}}.$$

The function $S(k)$ from (2) has a pole at $k_\star = -i\alpha/2$, which corresponds to

$$\frac{\sqrt{2mE_\star}}{\hbar} = -i\frac{\alpha}{2} \quad \to \quad \boxed{E_\star = -\frac{mg^2}{2\hbar^2} = E_0}.$$

Question 2:

Consider particles with energy $0 < E < V_0$ incident on a potential barrier given by

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

1. Find the eigenfunctions.
2. Is there a chance for particles to pass the barrier? Discuss the results, and the discrepancy with classical results.

Solution:

1. The Schrödinger equation reads

$$\begin{cases} -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi, & x < 0 \text{ and } x > d, \\ -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V_0\psi = E\psi, & 0 < x < d, \end{cases} \rightarrow \begin{cases} \frac{d^2\psi}{dx^2} = -k^2\psi, & x < 0 \text{ and } x > d, \text{ where } k \equiv \frac{\sqrt{2mE}}{\hbar} \quad \text{is real,} \\ \frac{d^2\psi}{dx^2} = \kappa^2\psi, & 0 < x < d, \text{ where } \kappa \equiv \frac{\sqrt{2m(V_0-E)}}{\hbar} \quad \text{is real.} \end{cases}$$

The solution to this equation is of the form

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & x < 0, \\ Ce^{\kappa x} + De^{-\kappa x}, & 0 < x < d, \\ Fe^{ikx} + Ge^{-ikx}, & x > d. \end{cases}$$

Assuming that the incident particle comes from the left we have $G = 0$. The boundary conditions read

$$\psi(0_-) = \psi(0_+): \quad A + B = C + D, \tag{1}$$
$$\psi'(0_-) = \psi'(0_+): \quad ik(A - B) = \kappa(C - D), \tag{2}$$
$$\psi(d_-) = \psi(d_+): \quad Ce^{\kappa d} + De^{-\kappa d} = Fe^{ikd}, \tag{3}$$
$$\psi'(d_-) = \psi'(d_+): \quad \kappa\left(Ce^{\kappa d} - De^{-\kappa d}\right) = ikFe^{ikd}. \tag{4}$$

At this point we leave explicit calculations and give the solution

$$B = -\frac{\left(\kappa^2 + k^2\right)\left(e^{\kappa d} - e^{-\kappa d}\right)}{(k - i\kappa)^2 e^{-\kappa d} + (\kappa - ik)^2 e^{\kappa d}} A,$$
$$C = -\frac{2k(k - i\kappa)e^{-\kappa d}}{(k + i\kappa)^2 e^{\kappa d} - (k - i\kappa)^2 e^{-\kappa d}} A,$$
$$D = \frac{2k(k + i\kappa)e^{\kappa d}}{(k + i\kappa)^2 e^{\kappa d} - (k - i\kappa)^2 e^{-\kappa d}} A,$$
$$F = \frac{4i\kappa k e^{-ikd}}{(k + i\kappa)^2 e^{\kappa d} - (k - i\kappa)^2 e^{-\kappa d}} A.$$

2. The transmission coefficient is $T = |J_t| / |J_i|$, where

$$J_i = \frac{\hbar}{m}\text{Im}\left[\psi_i^* \frac{\partial \psi_i}{\partial x}\right] = -\frac{\hbar k}{m}|A|^2,$$
$$J_t = \frac{\hbar}{m}\text{Im}\left[\psi_t^* \frac{\partial \psi_t}{\partial x}\right] = -\frac{\hbar k}{m}|F|^2,$$

hence

$$
\begin{aligned}
T &= \frac{|F|^2}{|A|^2} \\
&= \left|\frac{4i\kappa k e^{-ikd}}{(k+i\kappa)^2 e^{\kappa d} - (k-i\kappa)^2 e^{-\kappa d}}\right|^2 \\
&= \left|\frac{2i\kappa k e^{-ikd}}{(k^2-\kappa^2)\sinh(\kappa d) + 2ik\kappa\cosh(\kappa d)}\right|^2 \\
&= \left|\frac{\left(k^2-\kappa^2\right)\sinh(\kappa d) - 2ik\kappa\cosh(\kappa d)}{(k^2-\kappa^2)^2\sinh^2(\kappa d) + (2k\kappa)^2\cosh^2(\kappa d)} 2i\kappa k e^{-ikd}\right|^2 \\
&= \frac{(2k\kappa)^2}{(k^2-\kappa^2)^2\sinh^2(\kappa d) + (2k\kappa)^2\cosh^2(\kappa d)} \\
&= \frac{(2k\kappa)^2}{(k^4-2k^2\kappa^2+\kappa^4)\sinh^2(\kappa d) + 4k^2\kappa^2\left(1+\sinh^2(\kappa d)\right)} \\
&= \frac{(2k\kappa)^2}{(2k\kappa)^2 + (k^2+\kappa^2)^2\sinh^2(\kappa d)}.
\end{aligned}
$$

Plugging in the definitions

$$
2k\kappa = \frac{4m\sqrt{E(V_0-E)}}{\hbar^2} \quad \text{and} \quad k^2+\kappa^2 = \frac{2mV_0}{\hbar^2},
$$

we find

$$
\boxed{T = \left[1 + \frac{V_0^2\sinh^2(\kappa d)}{4E(V_0-E)}\right]^{-1}},
$$

hence, unlike the classical scenario, there is a chance to "tunnel" through the barrier! Note that in the limit $d \to \infty$ we get $T \to 0$ just like in the step potential.

Question 3:

Consider a particle with energy $-V_0 < E < 0$ moving inside a potential well by

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

Find a condition for calculating the possible energy levels for the particle.

Solution:

The Schrödinger equation reads

$$
\begin{cases} -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - V_0\psi = E\psi, & x < -a \text{ and } x > a, \\ -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi, & -a < x < a, \end{cases} \quad \to \quad \begin{cases} \frac{d^2\psi}{dx^2} = -k^2\psi, & x < -a \text{ and } x > a, \text{ where } k \equiv \frac{\sqrt{2m(E+V_0)}}{\hbar} \quad \text{is real,} \\ \frac{d^2\psi}{dx^2} = \kappa^2\psi, & -a < x < a, \text{ where } \kappa \equiv \frac{\sqrt{-2mE}}{\hbar} \quad \text{is real.} \end{cases}
$$

The solution to this equation is of the form

$$
\psi(x) = \begin{cases} Ae^{\kappa x} + Be^{-\kappa x}, & x < -a, \\ Ce^{ikx} + De^{-ikx}, & -a < x < a, \\ Fe^{\kappa x} + Ge^{-\kappa x}, & x > a. \end{cases}
$$

We require $B = F = 0$ so that ψ will remain finite at $x \to \pm\infty$, while the boundary conditions read

$$\begin{aligned}
\psi(-a_-) = \psi(-a_+): &\quad Ae^{-\kappa a} = Ce^{-ika} + De^{ika}, &(1)\\
\psi'(-a_-) = \psi'(-a_+): &\quad \kappa Ae^{-\kappa a} = ik\left(Ce^{-ika} - De^{ika}\right), &(2)\\
\psi(a_-) = \psi(a_+): &\quad Ce^{ika} + De^{-ika} = Ge^{-\kappa a}, &(3)\\
\psi'(a_-) = \psi'(a_+): &\quad ik\left(Ce^{ika} - De^{-ika}\right) = -\kappa Ge^{-\kappa a}. &(4)
\end{aligned}$$

Dividing the conditions yield

$$\begin{aligned}
\tfrac{(2)}{(1)}: &\quad \kappa = ik\tfrac{Ce^{-ika}-De^{ika}}{Ce^{-ika}+De^{ika}},\\
\tfrac{(4)}{(3)}: &\quad \kappa = ik\tfrac{-Ce^{ika}+De^{-ika}}{Ce^{ika}+De^{-ika}},
\end{aligned} \quad \to \quad C^2 - \cancel{DC\left(e^{2ika} - e^{-2ika}\right)} - D^2 = -C^2 - \cancel{DC\left(e^{2ika} - e^{-2ika}\right)} + D^2,$$

thus

$$C^2 = D^2 \quad \to \quad C = \pm D.$$

The two possible relations correspond to *even* and *odd* solutions

$$\psi(-a \le x \le a) = D\cos(kx) \quad \text{and} \quad \psi(-a \le x \le a) = D\sin(kx).$$

This could be anticipated by recalling that symmetric potentials must have either even and odd solutions. Thus, we may find the solution on one side and immediately get $\psi(-x) = \pm\psi(x)$. For the even solution ($C = D$, i.e. cosine function), we get

$$\psi(x) = \begin{cases} Ge^{-\kappa x}, & x > a, \\ D\cos(kx), & 0 < x < a, \\ \psi(-x), & x < 0, \end{cases}$$

with

$$\kappa = ik\frac{-e^{ika} + e^{-ika}}{e^{ika} + e^{-ika}} = k\tan(ka).$$

This equation determines the allowed energies. We may define

$$z \equiv ka, \quad \text{and} \quad z_0 \equiv a\sqrt{k^2 + \kappa^2} = \frac{a}{\hbar}\sqrt{2mV_0},$$

so that

$$\kappa a = \sqrt{z_0^2 - z^2}.$$

Then the equation for the allowed energies reads

$$\boxed{\tan z = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}}.$$

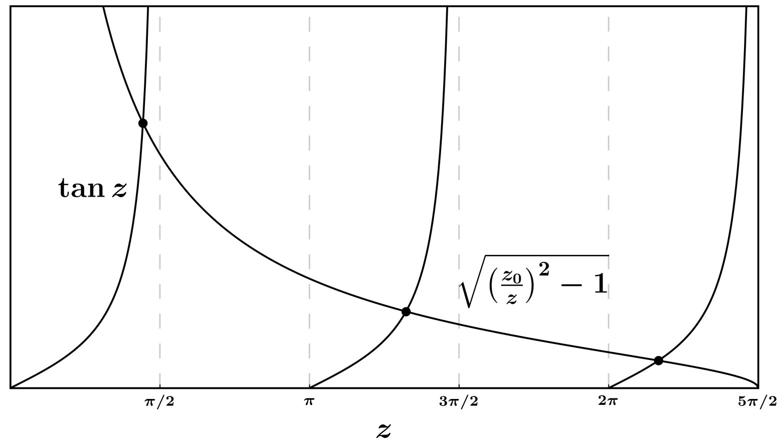
This is a transcendental equation for z (and hence for E) as a function of z_0 (i.e. the potential), than can be solved numerically, or graphically, by plotting both sides and search for the intersections. We can check the two interesting limits:

1. *Wide, deep well*: If $z_0 \gg z$ and is very large, then the right-hand-side is very large, thus

$$z_n \approx \frac{\pi}{2}(2n+1) \quad \to \quad E_n + V_0 \approx \frac{\pi^2\hbar^2(2n+1)^2}{2m(2a)^2} \quad (n = 0, 1, 2, \dots).$$

   This is exactly the (odd) energy levels in an infinite square well of width $2a$.

2. *Shallow, narrow well*: As z_0 decreases there are fewer bound states (the value for which $z_0/z = 1$ shifts left) up to $z_0 < \pi/2$, where we are left with a single bound state.



In a similar manner, for the odd solution we get

$$\psi(x) = \begin{cases} Ge^{-\kappa x}, & x > a, \\ D\sin(kx), & 0 < x < a, \\ \psi(-x), & x < 0, \end{cases}$$

with

$$\kappa = -ik\frac{e^{ika} + e^{-ika}}{e^{ika} - e^{-ika}} = -k\cot(ka).$$

So that the equation for the allowed energies reads

$$\boxed{-\cot z = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}}.$$

We can check the two interesting limits:

1. *Wide, deep well*: If $z_0 \gg z$ and is very large, then the right-hand-side is very large, thus

$$z_n \approx \pi n \quad \rightarrow \quad E_n + V_0 \approx \frac{\pi^2\hbar^2 n^2}{2ma^2} \quad (n = 1, 2, \dots).$$

   This is exactly the (even) energy levels in an infinite square well of width $2a$.

2. *Shallow, narrow well*: As z_0 decreases there are fewer bound states (the value for which $z_0/z = 1$ shifts left) up to $z_0 < \pi/2$, where we are left with no possible solution.

Together the two solutions make up all allowed the energies of the system.