Problem 1: Scattering by an attractive well

Refer to the solution we got in Problem Set 5 for scattering off a barrier. If we set up equations for the wave function in the three different regions, we see that this problem is identical to problem 4 of Problem Set 5, except for a new definition of q: $q = \sqrt{2m(E+V_o)}/\hbar$ since we now have a potential well instead of a barrier. The transmission coefficient is

$$T = \frac{4q^2k^2}{4q^2k^2 + \left(\frac{2mV_o}{\hbar^2}\right)^2 sin^2 2qa} \tag{1}$$

A plot of the transmission coefficient shows that the transmissivity goes to 1 at large energy, corresponding to the classical limit, and has regularly spaced (in terms of k) resonances for which $T = 1$ even at low energies.

Problem 2: Model for molecular potential

we have to solve the Schroedinger equation with a potential given by

$$U(x) = U_o\delta(x + \frac{a}{2}) + U_o\delta(x - \frac{a}{2}), U_o < 0. \tag{2}$$

We are looking for bound states, i.e. states with energy $E < 0$. Since $U(x) = 0$ away from the delta functions, the general form of the solution in each of the three regions is

$$\psi(x) = Ae^{kx} + Be^{-kx}, k = \sqrt{-2mE/\hbar^2} \tag{3}$$

However, in order to have a normalizable wave function, we must have $\psi(x) = Ae^{kx}$ for $x < -a/2$, and similarly $\psi(x) = De^{-kx}$ for $x > a/2$.

We can also take advantage of the symmetry of the potential to simplify the form of the wave function. Notice that the potential is even: $U(x) = U(-x)$. If you go to the corresponding Schroedinger equation and try setting $x = -x$, you'll see that the only possible solutions are those that satisfy either $\psi(x) = \psi(-x)$ or $\psi(x) = -\psi(-x)$. In other words, our eigenfunctions (solutions of the Schrodinger equation) must be either odd or even as well.

Even solutions

Let's look at even solutions first. Our symmetry requrement means that the wave function has the following form in the three regions of the problem:

$$\psi_1(x) = Ae^{kx} \qquad x < -\tfrac{a}{2} \tag{4}$$

$$\psi_2(x) = B\ cosh\ kx \quad -\tfrac{a}{2} < x < \tfrac{a}{2} \tag{5}$$

$$\psi_3(x) = Ae^{-kx} \qquad x > \tfrac{a}{2} \tag{6}$$

We only need to study the matching conditions at one of the delta functions; we would get exactly the same equations if we used the other one. The condition that the wave function be continuous gives

$$A\ e^{-ka/2} = B\ cosh\frac{ka}{2}. \tag{7}$$

The presence of the delta function (see problem 3) means that the derivative of the wave function has a discontinuity at $x = \pm a/2$:

$$\begin{aligned}
\psi_2'(-\frac{a}{2}) - \psi_1'(-\frac{a}{2}) &= \frac{2m}{\hbar^2} U_o \psi(-\frac{a}{2}), & (8)\\
-kB\ sinh\frac{ka}{2} - kAe^{-ka/2} &= \frac{2m}{\hbar^2} U_o A e^{-ka/2}, & (9)\\
-B\ sinh(\frac{ka}{2}) &= Ae^{-ka/2}\left(1 + \frac{2mU_o}{\hbar^2}\frac{1}{k}\right) & (10)\\
&= Ae^{-ka/2}\left(1 - \frac{\gamma}{ka}\right), & (11)
\end{aligned}$$

where

$$\gamma = -\frac{2mU_o a}{\hbar^2} > 0 \tag{12}$$

is a dimensionless constant that depends on the parameters of the problem.

Dividing, we get

$$tanh\frac{ka}{2} = \frac{\gamma}{ka} - 1. \tag{13}$$

This transcendental equation gives us the condition on k, and therefore the energy of the corresponding state. Let $z \equiv ka/2$, so that $ka = 2z$, and plot $tanh\ z$ and $\gamma/2z - 1$ on the same axes. You will see that there is always exactly one interesection point for nonzero γ. That means that there is always just one even solution to the Schroedinger equation for this problem.

Odd solutions

For the odd solutions we have $B = 0$. The continuity condition is

$$Ae^{-ka/2} = -C\ sinh\frac{ka}{2}, \tag{14}$$

and the cusp condition on the derivative at the delta function leads to

$$kC\ cosh\frac{ka}{2} - kAe^{-ka/2} = \frac{2m}{\hbar^2} U_o A e^{-ka/2}. \tag{15}$$

Dividing these two equations, we get, analogous to Eq. 13,

$$coth\ z = \frac{\gamma}{2z} - 1 \tag{16}$$

with the same substitions for z and γ. Rearranging Eq. 16, and using the definition of $coth\ z$, we find the following:

$$\begin{aligned}
coth\ z &= \frac{cosh\ z}{sinh\ z} = \frac{e^z + e^{-z}}{e^z - e^{-z}}; & (17)\\
\frac{\gamma}{2z} &= 1 + coth\ z = \frac{2e^z}{e^z - e^{-z}}, & (18)
\end{aligned}$$

$$\begin{aligned} \frac{2z}{\gamma} &= \frac{e^z - e^{-z}}{2e^z} && (19) \\ \frac{4}{\gamma}z &= 1 - e^{-2z}. && (20) \end{aligned}$$

The left-hand side is a line with slope $4/\gamma$; the slope of the expression on the right-hand side equals 2 at $z = 0$ and is monotonically decreasing. That means that this equation only has a solution when

$$\begin{aligned} \frac{4}{\gamma} &< 2, \text{or} && (21) \\ \gamma &> 2. && (22) \end{aligned}$$

We have found that a bound state ($E < 0$) exists only for sufficiently large γ. Referring to Eq. 12, we see that this corresponds to U_o or a being large, i.e. strongly attractive wells placed some distance apart.

If we again plot both sides of Eq. 16, we find that, for sufficiently large γ, that there is just one solution. If we plot both Eqs. 13 and 16, we will see that the intersection corresponding to the even wave function always occurs at a *higher* z-value, and therefore a greater absolute value of the energy, than the intersection point for the odd wave function (if one even exists). Since these energies are negative, that means that the even wave function is always the ground state of this system, while the odd wave function always lies higher in energy, and may not even correspond to a bound state.

Physically, this problem corresponds to a very simple model of an H_2^+ molecule, with two protons separated by a distance a and one electron binding them together. From a sketch of the two wave functions, it is apparent that the probability of finding the electron *between* the two protons is greater for the even wave function than for the odd one. When the electron is between the two protons, it can hold the system together. In constrast, when the electron is in the odd state, it can't shield as effectively the electrostatic repulsion between the protons. That's why the system is unstable (no bound state exists) for small a.

Wave function

All that remains to be done is to calculate the actual wave function. For each wave function we have three unknowns (A, B or C, and k), and three constraint equations: two from the matching condition, plus the requirement that the whole wave function be normalized. By now you should all know how, in principle, to compute normalization and solve for the coefficients of the wave function. I'm not going to work that out here because it's tedious and not particular illuminating. We were fortunate to have been able to find the energies and the types of solutions without going to much trouble.

Problem 3: Tunneling of various sorts

We want to find stationary states for particles scattering off the potential

$$U(x) = U_o\delta(x), U_o > 0. \tag{23}$$

We describe the incident particles as plane waves with wave function e^{ikx}, with $k > 0$.

a) Disconcontinuity of first derivative

Normally, wave functions are continuous and have continuous first derivatives. However, we can show that wave functions have a discontunity in their slope if the potential contains any delta-functions.

For generality, let suppose we have a delta function centered at the point $x = a$, so that $U(x) = U_o\delta(x - a)$. Put this potential into the Schroedinger equation. Now integrate each term in a very small neighborhood around $x = a$. We have

$$
\begin{aligned}
-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + \delta(x-a)\psi(x) &= E\psi(x), &(24)\\
\int_{a-\epsilon}^{a+\epsilon} -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x)dx + \int_{a-\epsilon}^{a+\epsilon} \delta(x-a)\psi(x)dx &= \int_{a-\epsilon}^{a+\epsilon} E\psi(x)dx, &(25)\\
-\frac{\hbar^2}{2m}\int_{a-\epsilon}^{a+\epsilon} \frac{d}{dx}\left(\frac{d\psi(x)}{dx}\right) + \psi(a) &= 0, &(26)\\
\psi'(a+\epsilon) - \psi'(a-\epsilon) &= \frac{2m}{\hbar^2}U_o\psi(a). &(27)
\end{aligned}
$$

We get the $\psi'(x)$ terms from the fundamental theorem of calculus. For the integral with the delta function the rule is evaluate everything in the integral at the point or points for which the argument in the delta function is zero. The term on the right hand side is zero because the wave function is continuous; for arbitrarily small ϵ the area under $\psi(x)$ is zero. Thus we see that if we take the difference of the slope of the wave function to the left of the delta function and the slope of the wae function to the right, the result is not zero; hence there is a discontinuity in the slope at that point.

b) Derive the wave function.

In the two regions we have

$$\psi_1(x) = e^{ikx} + re^{-ikx} \quad x < 0 \tag{28}$$

$$\psi_2(x) = te^{ikx} \quad x > 0 \tag{29}$$

Enforcing continuity and the derivative cusp condition at $x = 0$, we obtain the equations

$$
\begin{aligned}
1 + r &= t, &(30)\\
ikt - (ik - ikr) &= \frac{2mU_o}{\hbar^2}t. &(31)
\end{aligned}
$$

Solving, we get

$$
\begin{aligned}
t &= \left(1 - \frac{mU_o}{i\hbar^2 k}\right)^{-1}, &(32)\\
r &= t - 1. &(33)
\end{aligned}
$$

c) Transmission coefficient.

$$
\begin{aligned}
T &= |t|^2 && (34)\\
&= \left(1+\frac{m^2U_o^2}{\hbar^4k^2}\right)^{-1} && (35)\\
&= \left(1+\frac{m}{2\hbar^2}\frac{U_o^2}{E}\right)^{-1}, && (36)
\end{aligned}
$$

where we used $E = \hbar^2k^2/2m$.
d) Delta function barrel.

The potential is

$$
U(x) = U_o\delta(x) + U_o\delta(x-a), U_o > 0. \quad (37)
$$

We have electrons incident from the left, with positive energies, so that the wave function in the three regions is

$$
\begin{aligned}
\psi_1(x) &= e^{ikx} + re^{-ikx} \qquad x < 0 && (38)\\
\psi_2(x) &= Ae^{ikx} + Be^{-ikx} \quad 0 < x < a && (39)\\
\psi_3(x) &= te^{ikx} \qquad x > a && (40)
\end{aligned}
$$

We have four unknown parameters: A, B, r, and t. We will obtain four equations relating these unknowns, two each from the two matching conditions at the delta functions.

The requirement of continuity at $x = 0$ and $x = a$ gives us

$$
\begin{aligned}
1 + r &= A + B \text{ and} && (41)\\
te^{ika} &= Ae^{ika} + Be^{-ika}. && (42)
\end{aligned}
$$

The cusp in the first derivative gives

$$
\begin{aligned}
ik(A-B) - ik(1-r) &= \frac{2mU_o}{\hbar^2}(1+r) \text{ and} && (43)\\
ikte^{ika} - ik(Ae^{ika} - Be^{-ika} &= \frac{2mU_o}{\hbar^2}te^{ika}. && (44)
\end{aligned}
$$

At this point I found it helpful to make the substitutions

$$
\begin{aligned}
\alpha &\equiv e^{-2ika}, && (45)\\
q &\equiv \frac{2mU_o}{i\hbar^2}. && (46)
\end{aligned}
$$

Now we have the tidy set of four equations

$$\begin{aligned} 1+r &= A+B && (47)\\ t &= A+\alpha B && (48)\\ A-B &= 1-r+\frac{q}{k}(1+r) && (49)\\ T &= A-\alpha B+\frac{q}{k}t && (50) \end{aligned}$$

I punched these equations into Mathematica, and obtained

$$\begin{aligned} r &= \frac{q(2k+2\alpha k+q-\alpha q)}{4\alpha k^2-4\alpha kq-q^2+\alpha q^2} && (51)\\ t &= \frac{4\alpha k^2}{4\alpha k^2-4\alpha kq-q^2+\alpha q^2} && (52)\\ A &= \frac{2\alpha k(2k-q)}{4\alpha k^2-4\alpha kq-q^2+\alpha q^2} && (53)\\ B &= \frac{2kq}{4\alpha k^2-4\alpha kq-q^2+\alpha q^2}. && (54) \end{aligned}$$

e) Transmission coefficient

Making the back-substitions, we have

$$t=\frac{\hbar^4k^2}{\hbar^4k^2+2imU_o\hbar^2k-m^2U_o^2+e^{2ika}m^2U_o^2} \tag{55}$$

The modulus squared of t is then

$$T=\frac{\hbar^8k^4}{(\hbar^4k^2-m^2U_o^2+m^2U_o^2cos\ 2ka)^2+(2m\hbar^2kU_o+m^2U_o^2sin\ 2ka)^2}. \tag{56}$$

I used Mathematica to graph this, using the substitutions $\hbar\rightarrow 1, m\rightarrow 1, U_o\rightarrow 1, a\rightarrow 2$, and plotting vs. k from .01 to 10.

See the accompanying Mathematica notebook for the rest of the solution.

Problem 4: Bound states of a square well potential

a) Wave function

We need to find the wave function in the three regions. For the two regions outside the box, we need decaying exponentials since the energy is less than the potential energy there ($E<0$). Inside the box, however, $E>-U_o$, so the wave function must be a linear combination of sines and cosines. We can write this as

$$\begin{aligned} \psi_1(x) &\propto e^{kx} && x\le a && (57)\\ \psi_2(x) &\propto Acos\ qx+Bsin\ qx && -a<x<a && (58)\\ \psi_3(x) &\propto e^{-kx} && x\ge a && (59) \end{aligned}$$

where

$$k = \frac{\sqrt{-2mE}}{\hbar} \text{ and} \tag{60}$$

$$q = \frac{\sqrt{2m(U_o + E)}}{\hbar}. \tag{61}$$

For stationary states, the complete, time-dependent wave function is given by

$$\psi(x,t) = \psi(x)e^{-iEt/\hbar}. \tag{62}$$

We need to show that our wave functions satisfy the time-dependent Schroedinger equation

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + U(x)\psi(x,t). \tag{63}$$

Plugging in our definition of $\psi(x,t)$, we see that the left hand side of Eq. 63 is always equal to $E\psi(x,t)$. For the right-hand side, we get:

$$\text{Region 1}: \quad -\tfrac{\hbar^2}{2m}k^2\psi(x,t) + 0 \tag{64}$$

$$= -\tfrac{\hbar^2}{2m}\left(\tfrac{-2mE}{\hbar^2}\right)\psi(x,t) \tag{65}$$

$$= E\psi(x,t) \tag{66}$$

$$\text{Region 2}: \quad -\tfrac{\hbar^2}{2m}(-q^2)\psi(x,t) - U_o\psi(x,t) \tag{67}$$

$$= -\tfrac{\hbar^2}{2m}\left(-\tfrac{2m}{\hbar^2}(U_o + E)\right)\psi(x,t) - U_o\psi(x,t) \tag{68}$$

$$= E\psi(x,t) \tag{69}$$

$$\text{Region3 : Same as Region 1.} \tag{70}$$

b) Finding the solutions

For the even solutions we have

$$\psi_1(x) = Ce^{kx} \tag{71}$$

$$\psi_2(x) = A\cos qx \tag{72}$$

$$\psi_3(x) = Ce^{-kx} \tag{73}$$

The matching conditions are

$$Ce^{-ka} = A\cos qa \text{ and} \tag{74}$$

$$kCe^{-ka} = Aq\sin qa. \tag{75}$$

Dividing and rearranging terms, we obtain

$$k = q\tan qa; \tag{76}$$

$$\tan qa = \frac{k}{q} \tag{77}$$

$$= \sqrt{\frac{k^2}{q^2}} \tag{78}$$

$$= \frac{\sqrt{\frac{-2mE}{\hbar^2}}}{q} \tag{79}$$

$$= \frac{\sqrt{\left(\frac{-2mE}{\hbar^2} + \frac{2mU_o}{\hbar^2} - \frac{2mU_o}{\hbar^2}\right) a^2}}{qa} \tag{80}$$

$$= \frac{\sqrt{c^2 - q^2a^2}}{qa}\ ,\ c^2 \equiv \frac{2mU_o a^2}{\hbar^2}. \tag{81}$$

For the odd solutions, we have

$$\psi_1(x) = Ce^{kx} \tag{82}$$

$$\psi_2(x) = Bsin\ qx \tag{83}$$

$$\psi_3(x) = -Ce^{-kx} \tag{84}$$

Continuity of the wave function and its first derivative give

$$Ce^{-ka} = -Bsin\ qa \tag{85}$$

$$kCe^{-ka} = qBcos\ qa \tag{86}$$

Diving, we get

$$\frac{1}{k} = -\frac{1}{q} tan\ qa \tag{87}$$

so that

$$tan\ qa = -\frac{q}{k} = -\frac{qa}{\sqrt{c^2 - q^2a^2}}. \tag{88}$$

Part c)

Supose $c = 3\pi + 1$. If we define $\chi \equiv qa$, then the energies for the even solutions correspond to solutions of the equation

$$tan\ \chi = \frac{\sqrt{(3\pi+1)^2 - \chi^2}}{\chi} = \sqrt{\left(\frac{3\pi+1}{\chi}\right)^2 - 1}. \tag{89}$$

The energies for the odd solutions correspond to solutions of

$$-\ cot\ \chi = \sqrt{\left(\frac{3\pi+1}{\chi}\right)^2 - 1}. \tag{90}$$

The right hand sides of Eqs. 89-90 go to zero at $\chi = 3\pi + 1$, so it's easy from a graph of these two equations that there are four even states and three odd states.

The rest of this problem is explained in the accompanying Mathematica notebook.