1. **a)** *Consider a particle in one dimension, with the potential*

$$V(x) = -g(\delta(x+a) + \delta(x-a)) \ ,$$

where $\delta(x)$ is the Dirac delta function and $g > 0$. Find the ground state energy in terms of m, g, a and $\hbar$.

Correction: I didn't realize when I assigned this, that solving for the ground state energy involved solving a transcendental equation (which cannot be solved analytically). So just set up the equation you need to solve for the energy, and show how you can solve it graphically, similar to our treatment of the finite square well.

We can define three regions: region I is for $x < -a$; region II is for $0 < |x| < a$, and region III is for $x > a$. We are looking for a bound state which means $E < 0$, since $V(x) = 0$ for $x = \pm\infty$ in this problem. Define

$$\kappa \equiv \sqrt{2m|E|}/\hbar \ .$$

Then the general solution which does not blow up at $x = \pm\infty$ is

$$u(x) = \begin{cases} Ae^{\kappa x} & \text{Region I} \\ B\cosh\kappa x + C\sinh\kappa x & \text{Region II} \\ De^{-\kappa x} & \text{Region III} \end{cases} \tag{1}$$

Since we are interested in the ground state energy, we can simplify our life by only considering even parity solutions:

$$u(x) = \begin{cases} Ae^{\kappa x} & \text{Region I} \\ B\cosh\kappa x & \text{Region II} \\ Ae^{-\kappa x} & \text{Region III} \end{cases} \tag{2}$$

Now we need only consider the boundary conditions at $x = a$ or $x = -a$, but not both. I will consider only $x = a$.

The boundary conditions for a δ-function potential, as discussed in class, are:

$$u_{II}(a) = u_{III}(a) \ , \tag{3}$$

and

$$-\frac{\hbar^2}{2m}\left(u'_{III}(a) - u'_{II}(a)\right) - g u_{III}(a) = 0 \ . \tag{4}$$

Defining

$$\kappa_0 \equiv \frac{2mg}{\hbar^2} \ ,$$

the second boundary condition reads:

$$u'_{III}(a) - u'_{II}(a) = \kappa_0 u_{III}(0) \ . \tag{5}$$

Plugging in our general solution to these equations, we get:

$$B\cosh\kappa a \quad = \quad A e^{-\kappa a} \ , \tag{6}$$

and

$$-\kappa A e^{-\kappa a} - \kappa B \sinh\kappa a = \kappa_0 A e^{-\kappa a} \quad \Longrightarrow \quad B\kappa \sinh\kappa a = A(\kappa_0 - \kappa) e^{-\kappa a} \ . \tag{7}$$

Dividing eq. (7) by eq. (6) gives a transcendental equation for κ (and hence the binding energy $|E|$):

$$\tanh\kappa a = \frac{\kappa_0 - \kappa}{\kappa} \ , \tag{8}$$

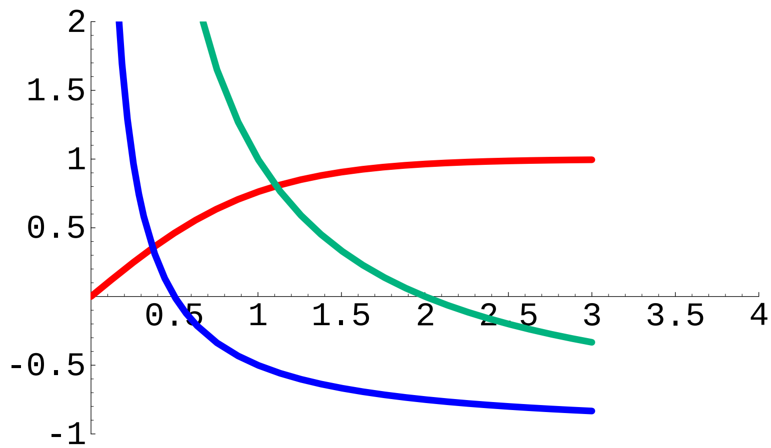
To solve this graphically, multiply the top and bottom of the right side of the above equation by a, and define

$$z \equiv \kappa a = a\sqrt{2m|E|}/\hbar \ , \qquad z_0 = \kappa_0 a = \frac{2mga}{\hbar^2} \ , \tag{9}$$

so that

$$\tanh z = \frac{z_0 - z}{z} \ . \tag{10}$$

Then plot the functions $\tanh z$ (red) and $\frac{z_0 - z}{z}$ for various z_0. See plot below for $z_0 = .5$ (blue) and $z_0 = 2$ (green):



Where the red curve ($tanh$) intersects the blue or green curves ($\frac{z_0-z}{z}$), given some number $z_0 = 2mga/\hbar^2$, that value for z is your solution, and you can find $|E| = \frac{\hbar^2}{2m}(z/a)^2$.

b) *How does the ground state energy change as you increase a? Consider the analogous problem where the delta functions are replaced by finite square wells. Without solving any equations argue from the uncertainty principle why the ground-state energy will go up with the separation of the two square wells by comparing the cases when the square wells are touching each other, to when the are infinitely separated. This can be considered as a crude model for certain types of molecular binding; the delta functions or square wells can represent atoms at separation $2a$ to which an electron is attracted. The sharing of the electron between the two atoms gives rise to the binding force you have found.*

Correction: You should be able to show that for large separation a, the binding energy goes to a constant (why?). You should also be able to show that for small separation a, the binding energy decreases as a increases.

Note for very large z_0, corresponding to large separation a, the tanh curve will equal one in that region, and we get the solution $\frac{z_0-z}{z} = 1$, or $z = z_0/2$, implying for the energy

$$E = -\frac{g^2 m}{2} \quad (a \to \infty) \ , \tag{11}$$

which is just the binding energy for a particle in a *single* δ-function potential, $V(x) = -g\delta(x)$. This makes sense when the δ-functions are infinitely separated.

For small separation ($z0 \ll 1$) we can Taylor expand our transcendental equation eq. (8) to get

$$(z_0 - z) = z \tanh z = 0 + O(z^2) \qquad \Longrightarrow \qquad z = z_0 + O(z_0^2) \tag{12}$$

or

$$E = -2g^2 m \quad (a \to 0) \tag{13}$$

This is the binding energy for a particle in a single δ-function potential $V(x) = -2g\delta(x)$ (which is what you get if $a \to 0$ so that $-g\delta(x+a)$ and $-g\delta(x-a)$ are sitting on top of each other) and is $4\times$ the binding energy that we got for $a \to \infty$.

To see the a dependence of the energy for small a it is necessary to expand eq. (8) to one further order:

$$(z_0 - z) = z \tanh z = z^2 + O(z^4) \qquad \Longrightarrow \qquad z = z_0 - z_0^2 + O(z_0^3) \tag{14}$$

or

$$E = 2g^2 m \left(-1 + 4agm/\hbar^2 + \ldots\right) \tag{15}$$

which shows the binding energy $|E|$ decreasing as a increases.

Finally, with a little algebra, one can show directly by differentiating both sides of eq. (8) with respect to a, that $d|E|/da$ is always negative for positive a, meaning that the binding energy decreases monotonically with the separation a.

⋆ **2.** *Consider a step potential in one dimension,*

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

Sketch this potential (assume $V_0 > 0$). Assume a beam of particles is incident heading in the $+x$ direction, originating from $x = -\infty$, with energy E. Compute the reflection and transmission probabilities as a function of $k \equiv \sqrt{2mE}/\hbar$ and $k' \equiv \sqrt{2m(E+V_0)}/\hbar$. What would the classical result be for the reflection probability?

Define $x < 0$ to be region I and $x > 0$ to be region II. Taking into account that no particles are coming in from the right, the general solution is

$$u(x) = \begin{cases} Ie^{ikx} + Re^{-ikx} & \text{Region I} \\ Te^{ik'x} & \text{Region II} \end{cases} \qquad k \equiv \frac{\sqrt{2mE}}{\hbar} , \quad k' \equiv \frac{\sqrt{2m(E+V_0)}}{\hbar} . \tag{16}$$

Then the boundary conditions are

$$u_I(0) = u_{II}(0) , \qquad u_I'(0) = u_{II}'(0) , \tag{17}$$

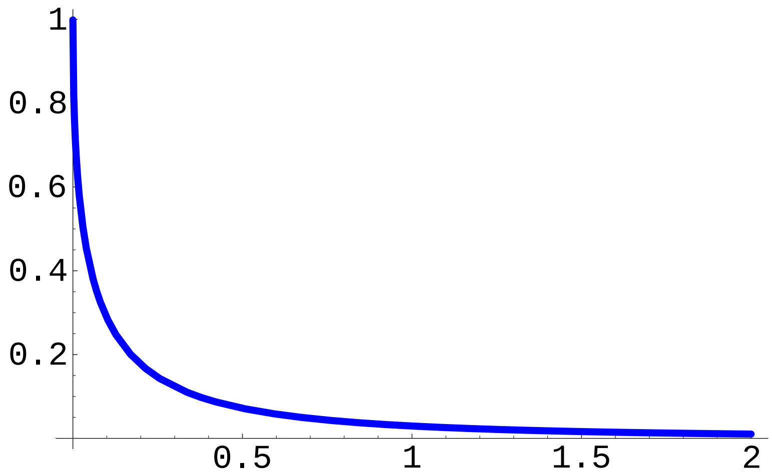
or

$$I + R = T , \qquad ik(I - R) = ik'T \tag{18}$$

with the solution for the reflection probability

$$P_R = \frac{|R|^2}{|I|^2} = \left|\frac{k-k'}{k+k'}\right|^2 = \left|\frac{\sqrt{\xi} - \sqrt{1-\xi}}{\sqrt{\xi} + \sqrt{1-\xi}}\right|^2 , \qquad \xi \equiv \frac{E}{V_0} . \tag{19}$$

A plot of P_R versus $\xi = E/V_0$ looks like:



Note that the reflection probability goes to zero for $E \gg V_0$, as it would classically; however, for E much smaller than V_0 we see almost total reflection!

3. *Gasiorowicz 11-2*

Using

$$x = r\sin\theta\cos\phi\ , \quad y = r\sin\theta\sin\phi\ , \quad z = r\cos\theta\ , \tag{20}$$

one finds

$$\begin{aligned} Y_{0,0} &= \sqrt{\frac{1}{4\pi}} \\ Y_{1,1} &= -\sqrt{\frac{3}{8\pi}}\frac{x+iy}{r} \\ Y_{1,0} &= \sqrt{\frac{3}{4\pi}}\frac{z}{r} \\ Y_{2,2} &= \sqrt{\frac{15}{32\pi}}\frac{(x+iy)^2}{r^2} \\ Y_{2,1} &= -\sqrt{\frac{15}{32\pi}}\frac{(x+iy)z}{r^2} \\ Y_{2,0} &= \sqrt{\frac{5}{16\pi}}\frac{3z^2-r^2}{r^2} \end{aligned} \tag{21}$$

In the above equations, $r = \sqrt{x^2+y^2+z^2}$.

The fact that all of these functions are invariant when you scale x, y and z (and hence r) by a common factor shows that they only depend on angles.

⋆ **4.** *Gasiorowicz 11-5*

Rewrite $L_x^2 + L_y^2 = L^2 - L_z^2$ so that

$$H = \frac{L^2 - L_z^2}{2I_1} + \frac{L_z^2}{2I_2} \; . \tag{22}$$

Evidently, the wavefunctions for the rotator (think of it as a dumbell, or a diatomic molecule with the distance between atoms being rigidly fixed) are just the $Y_{lm}(\theta, \phi)$, where θ and ϕ define the orientation of the rotator. The energies are the eigenvalues of H: energies

$$E_{\ell,m} = \hbar^2 \left(\frac{\ell(\ell+1) - m^2}{I_1} + \frac{m^2}{2I_2} \right) \; . \tag{23}$$

5. *Gasiorowicz 11-8*

We saw in class that

$$Y_{3,3} = N e^{3i\phi} \sin^3\theta \; . \tag{24}$$

We find the normalization by requiring

$$1 = \int_0^\pi d\theta \int_0^{2\pi} d\phi \sin\theta |Y_{3,3}|^2 = |N|^2 2\pi \int_0^\pi d\theta \sin^7\theta = \frac{64\pi}{35}|N|^2 \; , \tag{25}$$

so with the usual sign convention (negative N for odd ℓ) we get

$$Y_{3,3} = -\sqrt{\frac{35}{64\pi}} e^{3i\phi} \sin^3\theta \; . \tag{26}$$

To get the lower m values we apply L_-, using the relation discussed in class:

$$L_- Y_{\ell,m} = \hbar\sqrt{\ell(\ell+1) - m(m-1)} Y_{\ell,m-1} = \hbar e^{-i\phi} \left[-\partial_\theta + i\cot\theta\partial_\phi \right] Y_{\ell,m} \tag{27}$$

or

$$Y_{\ell,m-1} = \sqrt{\frac{1}{\ell(\ell+1) - m(m-1)}} e^{-i\phi} \left[-\partial_\theta + i\cot\theta\partial_\phi \right] Y_{\ell,m} \; . \tag{28}$$

Plugging in our function for $Y_{3,3}$ in eq. (26) we get

$$Y_{3,2} = -\sqrt{\frac{35}{64\pi}} \sqrt{\frac{1}{6}} (-6e^{2i\phi} \cos\theta \sin^2\theta) = \sqrt{\frac{105}{32\pi}} e^{2i\phi} \cos\theta \sin^2\theta \tag{29}$$

Applying eq. (28) to $Y_{3,2}$ to get $Y_{3,1}$, and then subsequently to $Y_{3,1}$ to get $Y_{3,0}$ yields the desired functions:

$$\begin{aligned}
Y_{3,3} &= -\sqrt{\frac{35}{64\pi}}e^{3i\phi}\sin^3\theta \ , \\
Y_{3,2} &= \sqrt{\frac{105}{32\pi}}e^{2i\phi}\sin^2\theta\cos\theta \\
Y_{3,1} &= -\sqrt{\frac{21}{64\pi}}e^{i\phi}\sin\theta(5\cos^2\theta - 1) \\
Y_{3,0} &= \sqrt{\frac{7}{16\pi}}(5\cos^3\theta - 3\cos\theta) \qquad (30)
\end{aligned}$$

I used Mathematica to make this less tedious...