

DOUBLE DELTA FUNCTION WELL

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Post date: 1 Aug 2012.

Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 2.27.

We can extend the case of the particle in a delta function well to the case of a particle in a double delta function well. That is, the potential is

$$V(x) = -\alpha [\delta(x+a) + \delta(x-a)] \quad (1)$$

where α gives the strength of the well.

Since the potential is an even function, any solution can be expressed as a linear combination of even and odd solutions. Consider even solutions first. In regions away from the delta functions, the Schrödinger equation is, since $V = 0$:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) = E\psi(x) \quad (2)$$

The most general even solution of this equation is (with $\kappa \equiv \sqrt{-2mE}/\hbar$; remember E is negative so κ is real)

$$\psi_e(x) = \begin{cases} Ae^{-\kappa x} & x > a \\ Be^{-\kappa x} + Ce^{\kappa x} & 0 < x < a \\ Be^{\kappa x} + Ce^{-\kappa x} & -a < x < 0 \\ Ae^{\kappa x} & x < -a \end{cases} \quad (3)$$

We can narrow down the number of constants by applying Born's conditions. At all points the wave function must be continuous, so applying this condition at $x = a$ gives

$$Ae^{-\kappa a} = Be^{-\kappa a} + Ce^{\kappa a} \quad (4)$$

$$A = B + Ce^{2\kappa a} \quad (5)$$

At $x = 0$, the continuity condition gives us no information, and at $x = -a$ we just repeat the condition at $x = a$.

Another condition is that the derivative of the wave function must be continuous at all points where the potential is finite. This means we can apply this condition at $x = 0$ to get

$$-B\kappa + C\kappa = B\kappa - C\kappa \quad (6)$$

$$C - B = B - C \quad (7)$$

$$B = C \quad (8)$$

Thus we get

$$\psi_e(x) = \begin{cases} B(1 + e^{2\kappa a})e^{-\kappa x} & x > a \\ B(e^{-\kappa x} + e^{\kappa x}) & -a < x < a \\ B(1 + e^{2\kappa a})e^{\kappa x} & x < -a \end{cases} \quad (9)$$

The constant B could be found by normalizing the wave function but we won't need to do that to find the energies.

Following the same logic as in the single delta function well, we calculate the difference in the derivative across the delta function at $x = a$. We get

$$\psi'_{e(a+)} = -B\kappa(1 + e^{2\kappa a})e^{-\kappa a} \quad (10)$$

$$\psi'_{e(a-)} = B(-\kappa e^{-\kappa a} + \kappa e^{\kappa a}) \quad (11)$$

$$= -B\kappa e^{-\kappa a}(1 - e^{2\kappa a}) \quad (12)$$

The change in derivative across $x = a$ is then

$$\Delta\psi'_e = \psi'_{e(a+)} - \psi'_{e(a-)} \quad (13)$$

$$= -2B\kappa e^{\kappa a} \quad (14)$$

As in the single delta function well, we must also have

$$\Delta\psi'_e = -\frac{2m\alpha}{\hbar^2}\psi(a) \quad (15)$$

$$= -\frac{2m\alpha}{\hbar^2}B(e^{-\kappa a} + e^{\kappa a}) \quad (16)$$

$$\kappa = \frac{m\alpha}{\hbar^2}(1 + e^{-2\kappa a}) \quad (17)$$

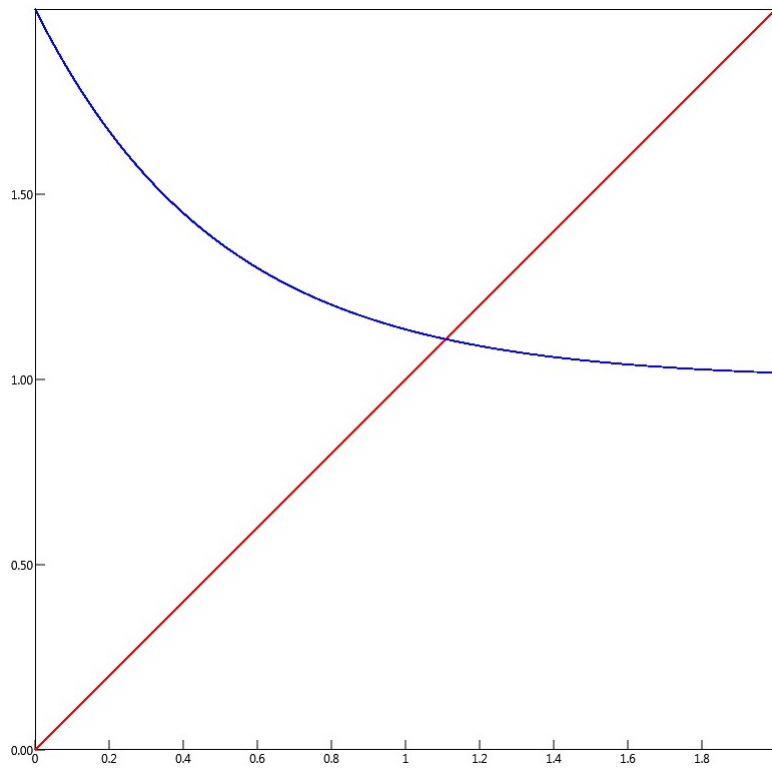
To get a condition on the energy, we need κ , but this is a transcendental equation in κ , so the only way we can solve it is numerically. We can see the solutions graphically, however, if we plot the left and right sides of the equation and look for intersections. To make this easier, we'll introduce the auxiliary variable $\xi \equiv a\kappa$ to get

$$\xi = \frac{ma\alpha}{\hbar^2} \left(1 + e^{-2\xi}\right) \quad (18)$$

Now if we specify α we can get a numerical solution. If $\alpha = \hbar^2/ma$, we get

$$\xi = \left(1 + e^{-2\xi}\right) \quad (19)$$

In the plot below, we draw $y = \xi$ in red and $y = (1 + e^{-2\xi})$ in blue.



We see there is a solution around $\xi = 1.1$, but to get this more accurately, we can use software like Maple's `fsolve` command to solve the equation numerically. We get $\xi = 1.108857553$. From this we can get the energy as

$$E = -\frac{\hbar^2 \kappa^2}{2m} \quad (20)$$

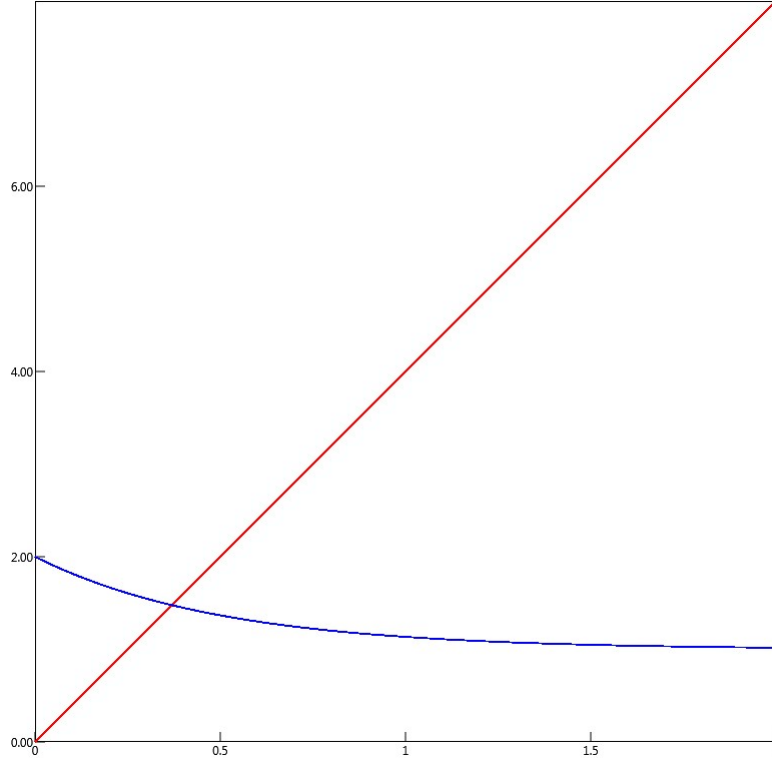
$$= -\frac{\hbar^2 \xi^2}{2ma^2} \quad (21)$$

$$= -0.614782 \frac{\hbar^2}{ma^2} \quad (22)$$

For $\alpha = \hbar^2/4ma$, the equation becomes

$$4\xi = (1 + e^{-2\xi}) \quad (23)$$

In the plot below, $y = 4\xi$ is in red and $y = (1 + e^{-2\xi})$ is in blue.



A solution exists around $\xi = 0.4$ and using Maple again we discover that $\xi = 0.3694175156$, giving an energy of $E = -0.068235\hbar^2/ma^2$.

For the odd solution, we start off with the most general odd wave function:

$$\psi_o(x) = \begin{cases} Ae^{-\kappa x} & x > a \\ Be^{-\kappa x} - Ce^{\kappa x} & 0 < x < a \\ -Be^{\kappa x} + Ce^{-\kappa x} & -a < x < 0 \\ -Ae^{\kappa x} & x < -a \end{cases} \quad (24)$$

As before, the continuity condition at $x = a$ gives us

$$Ae^{-\kappa a} = Be^{-\kappa a} - Ce^{\kappa a} \quad (25)$$

$$A = B - Ce^{2\kappa a} \quad (26)$$

This time the continuity of the derivative at $x = 0$ gives us nothing new, but the continuity of the wave function itself gives us

$$B - C = -B + C \quad (27)$$

$$B = C \quad (28)$$

Thus the function is

$$\psi_o(x) = \begin{cases} B(1 - e^{2\kappa a})e^{-\kappa x} & x > a \\ B(e^{-\kappa x} - e^{\kappa x}) & -a < x < a \\ -B(1 - e^{2\kappa a})e^{\kappa x} & x < -a \end{cases} \quad (29)$$

From here we follow the same argument as above.

$$\psi'_{o(a+)} = -B\kappa(1 - e^{2\kappa a})e^{-\kappa a} \quad (30)$$

$$\psi'_{o(a-)} = B(-\kappa e^{-\kappa a} - \kappa e^{\kappa a}) \quad (31)$$

$$= -B\kappa e^{-\kappa a}(1 + e^{2\kappa a}) \quad (32)$$

The change in derivative across $x = a$ is then

$$\begin{aligned} \Delta\psi'_o &= \psi'_{o(a+)} - \psi'_{o(a-)} \\ &= 2B\kappa e^{\kappa a} \end{aligned}$$

As in the single delta function well, we must also have

$$\Delta\psi'_o = -\frac{2m\alpha}{\hbar^2}\psi(a) \quad (33)$$

$$= -\frac{2m\alpha}{\hbar^2}B(e^{-\kappa a} - e^{\kappa a}) \quad (34)$$

$$\kappa = \frac{m\alpha}{\hbar^2}(1 - e^{-2\kappa a}) \quad (35)$$

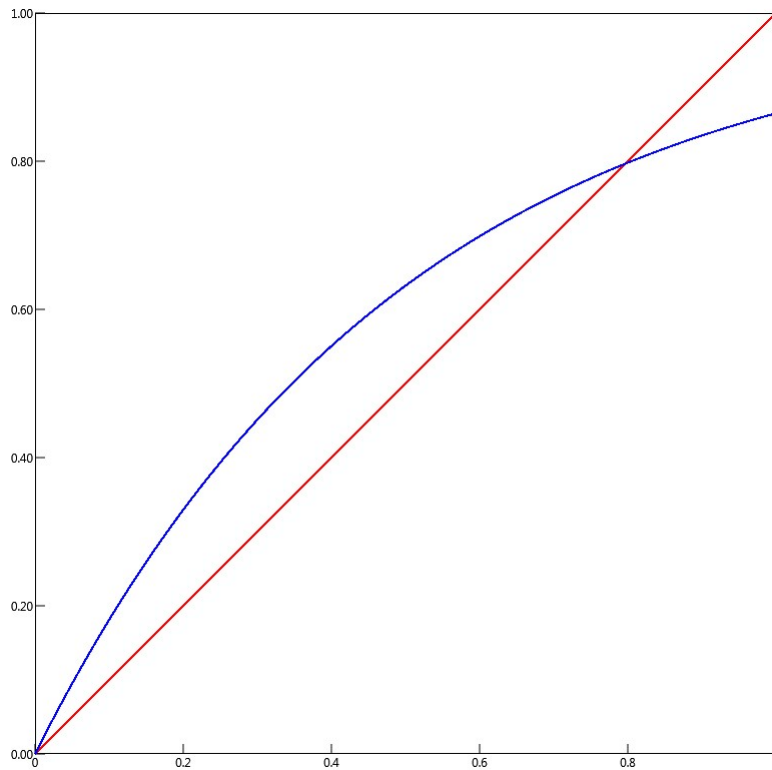
In terms of ξ we get

$$\xi = \frac{m\alpha}{\hbar^2}(1 - e^{-2\xi}) \quad (36)$$

If $\alpha = \hbar^2/ma$, we get

$$\xi = (1 - e^{-2\xi}) \quad (37)$$

In the plot below, we draw $y = \xi$ in red and $y = (1 - e^{-2\xi})$ in blue.



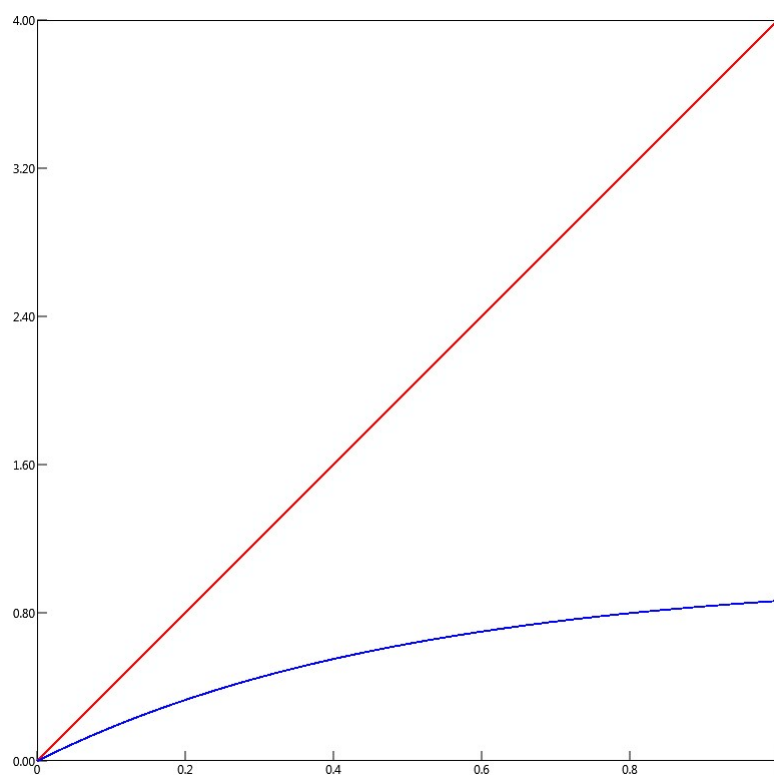
We see there is a solution near $\xi = 0.8$ and using Maple, we find $\xi = 0.79681213$, with corresponding energy $E = -0.317455\hbar^2/ma^2$.

There is also an intersection at $\xi = 0$ for any value of α . However, this would correspond to $E = 0$, which would mean that $d^2\psi/dx^2 = 0$ everywhere. This would imply $\psi(x) = Ax + B$ which isn't normalizable so it isn't a physically acceptable solution.

For $\alpha = \hbar^2/4ma$, the equation becomes

$$4\xi = (1 - e^{-2\xi}) \quad (38)$$

In the plot below, $y = 4\xi$ is in red and $y = (1 - e^{-2\xi})$ is in blue.



In this case, there is no intersection except the non-physical one at $\xi = 0$, so for this value of α , there is no bound state with an odd wave function.

PINGBACKS

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