Solving Schrödinger's equation: for a finite negative potential well

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Consider a finite potential well $U(x) = -q$ for $-a < x < a$ and $U(x) = 0$ otherwise for the Schrödinger equation. Find the discrete spectrum of bound states. Investigate wave functions behavior for several values of q and a. Is it possible to get potential well with a finite a that contains only one bound state?

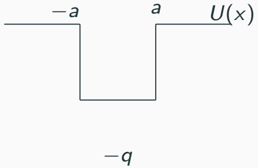


Figure 1: The graph of $U(x) = -q$ for $-a < x < a$ and $U(x) = 0$ otherwise.

Scientific Background

We can represent time-dependent Schrödinger equation as a second order PDE wave equation:

$$i\hbar\Psi_t = -\frac{\hbar}{2m}\Psi_{xx} + V(x)\Psi \text{ for } x \in \mathbb{R}, t \geq 0$$

where $\Psi = \Psi(x, t)$.

We can use the method of separation of variables and write

$$\Psi(x,t) = g(x)y(t)$$

where y is a solution to the equation

$$\frac{-\hbar^2}{2m}y'' + V(x)y = Ey.$$

Scientific Background

We split this up into three regions. If $x < -a$ then $U(x) = 0$. Then we have

$$\Psi'' + k^2\Psi = 0 \text{ where } k^2 = \frac{2mE}{\hbar^2}$$

Then the solutions are $\Phi(x) = A\cos(kx) + B\sin(kx)$ We may convert these to exponential functions, $y = Ae^{kx} + Be^{-kx}$.

Scientific Background

If $x \in [-a, a]$, then $U(x) = -q$. In this region the wave function takes the following form

$$\Psi'' - U(x)\Psi + k^2\Psi = 0 \text{ where } k^2 = \frac{2mE}{\hbar^2}$$

Recall that $U(x) = \frac{2m}{\hbar^2} V(x)$.

Let $\lambda^2 = \frac{2m(E+q)}{\hbar^2}$.

Then we have $\Psi'' + \lambda^2 \Psi = 0$.

So, we find $\Psi = C \sin(\lambda x) + D \cos(\lambda x)$.

Scientific Background

If $x > a$ then $U(x) = 0$. So, $y = Ee^{-kx} + Fe^{-kx}$ and is restricted to only one term because of the physical constraints of the system. In particular, the solution to the wave equation is square integrable. Therefore, we can omit the component that blows up to infinity.

Solution

Solution

$$y(x) = \begin{cases} Ae^{kx} + Be^{-kx} & x < -a \\ C\sin(\lambda x) + D\cos(\lambda x) & x \in [-a, a] \\ Ee^{kx} + Fe^{-kx} & x > a \end{cases}$$

The solutions to the wave equation are in the Hilbert space $\mathbb{L}^2$, e.g. the space of square integrable functions. Thus, as $x \to -\infty$ the term $Be^{-kx} \to \infty$ which contradicts square integrability. Therefore, $B = 0$. Similarly, as $x \to \infty$ we have $Ee^{k} \to \infty$ which implies $E = 0$. This yields a more applicable solution.

Solution

$$y(x) = \begin{cases} Ae^{kx} & x < -a \\ C\sin(\lambda x) + D\cos(\lambda x) & x \in [-a, a] \\ Fe^{-k} & x > a \end{cases}$$

Solution

Note that our well is symmetric around the origin, so we only have even solutions. Therefore, we may conclude that $C = 0$ since sin is an odd function.

Solution

$$y(x) = \begin{cases} Ae^{kx} & x < -a \\ D\cos(\lambda x) & x \in [-a, a] \\ Fe^{-k} & x > a \end{cases}$$

Solution

Because the first derivative of Schrödinger is continuous, we may examine the behaviour at the boundaries of the potential well to find solutions for the coefficients.

$$y(x) \xrightarrow[x \to -a]{} Ae^{-ka} = D\cos(-\lambda a) \tag{1}$$

$$y'(x) \xrightarrow[x \to -a]{} kAe^{-ka} = \lambda D\sin(-\lambda a) \tag{2}$$

$$y(x) \xrightarrow[x \to a]{} Fe^{-ka} = D\cos(\lambda a) \tag{3}$$

$$y'(x) \xrightarrow[x \to a]{} -kFe^{-ka} = -\lambda D\sin(\lambda a) \tag{4}$$

This yields four equations in four unknowns.

Solution

This yields four equations in four unknowns.

Dividing equation (2) by (1) we get

$$k = k\frac{Ae^{-ka}}{Ae^{-ka}} = \frac{\lambda D\sin(-\lambda a)}{D\cos(-\lambda a)} = \lambda\frac{\sin(-\lambda a)}{\cos(-\lambda a)} = \lambda\tan(-\lambda a)$$

Similarly, dividing equation (4) by (3) we get

$$-k = -k\frac{Fe^{-ka}}{Fe^{-ka}} = \frac{-\lambda D\sin(-\lambda a)}{D\cos(-\lambda a)} = -\lambda\frac{\sin(-\lambda a)}{\cos(-\lambda a)} = -\lambda\tan(-\lambda a)$$

Hence we get

$$k = \lambda\tan(\lambda a)$$

Solution

Since $k = \lambda \tan(\lambda a)$ we can multiply by a and substitute $z = \lambda a$ and get the form

Solution

$\frac{k}{\lambda} = \tan(z).$

Solution

Recall that $k^2 = \frac{2m|E|}{\hbar^2}$ and $\lambda^2 = \frac{2m}{\hbar^2}(E + V_0)$. Let $z_0^2 = \frac{2mV_0a^2}{\hbar^2}$. Then

$$\frac{k}{\lambda} = \sqrt{\frac{-2mE/\hbar^2}{z^2/a^2}} = \sqrt{\frac{-2mE/\hbar^2 a^2}{z^2}} = \sqrt{\frac{z_0^2 - z^2}{z^2}} = \sqrt{\frac{z_0^2}{z^2} - 1} = \sqrt{z_0^2 - z^2}$$

Then we get $tan(z) = \sqrt{z_0^2 - z^2}$.

Solution

This formula gives us the solutions to the even bound states of the wave equation.

Solution

$\tan(z) = \sqrt{z_0^2 - z^2}$ *where* $z = \lambda a$ *and* $z_0 = \frac{2mV_0 a^2}{\hbar^2}$.

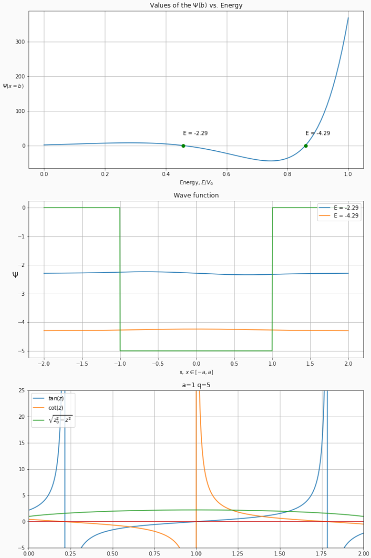
Now, because of parity we consider the odd solutions. After the same analysis above we get

Solution

$\cot(z) = \sqrt{z_0^2 - z^2}$ *where* $z = \lambda a$ *and* $z_0 = \frac{2mV_0 a^2}{\hbar^2}$.

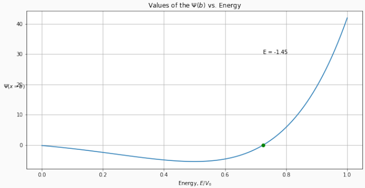
Solution

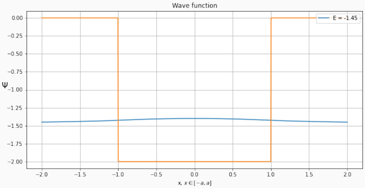
- Brent's method to find a zeros numerically.
- Runge Kutta we solve the wave equation.
- Graph for $\tan(z)$ and $\sqrt{z_0^2 - z^2}$ for $q = 5$ and $a = 1$.

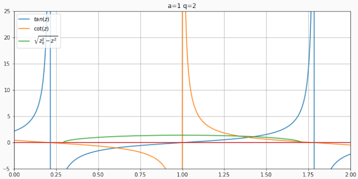


Solution

- Brent's method to find a zeros numerically.
- Runge Kutta we solve the wave equation.
- Graph for $\tan(z)$ and $\sqrt{z_0^2 - z^2}$ for $q = 2$ and $a = 1$.







Questions