

Attractive delta-function type potential
Masatsugu Sei Suzuki
Department of Physics, SUNY at Binghamton
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We discuss the 1D barrier problem in the presence of an attractive Dirac-delta function-type potential. This provides a simple model system for the bound state and transmission and reflection. When the energy of the particle is negative, we have a bound state. When the energy of the particle is positive, there occurs the transmission and reflection for the incident particle. For the bound state (the energy of the particle is negative), the wave function should be either an even function or an odd function, since the delta function potential is an even function. This property is discussed in terms of the parity operator.

1. Bound state ($E < 0$) in a delta function potential

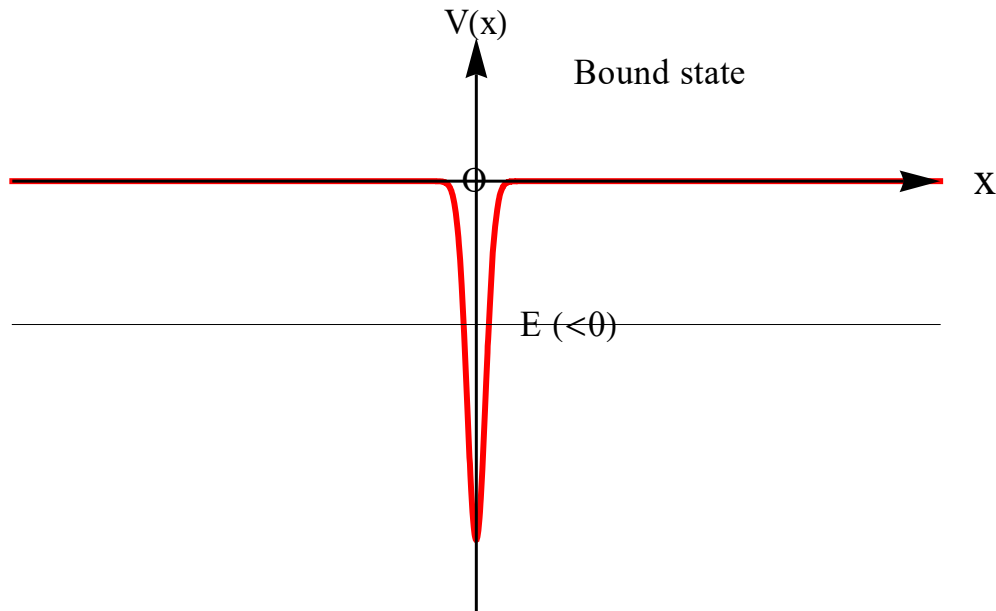


Fig. Bound state of the system (having the negative energy $E < 0$) in the presence of an attractive delta-function type potential.

We now consider a attractive potential of the form of Dirac delta function,

$$V(x) = -V_0\delta(x)$$

We find a bound state for the particle energy $E (< 0)$. The Schrödinger equation of this system is given by

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) - V_0 \delta(x) \psi(x) = E \psi(x).$$

Note that the unit of V_0 is [erg cm], but not [erg]. Integrating this equation between $-\varepsilon$ and $+\varepsilon$. Letting ε approach 0, we show that the derivative of the eigenfunction $\psi(x)$ presents a discontinuity at $x = 0$.

$$-\frac{\hbar^2}{2m} \int_{-\varepsilon}^{\varepsilon} \frac{d^2}{dx^2} \psi(x) dx - \int_{-\varepsilon}^{\varepsilon} V_0 \delta(x) \psi(x) dx = E \int_{-\varepsilon}^{\varepsilon} \psi(x) dx$$

or

$$-\frac{\hbar^2}{2m} \left(\frac{d\psi(x)}{dx} \right)_{x=\varepsilon} + \frac{\hbar^2}{2m} \left(\frac{d\psi(x)}{dx} \right)_{x=-\varepsilon} - V_0 \psi(0) \int_{-\varepsilon}^{\varepsilon} \delta(x) dx = E \int_{-\varepsilon}^{\varepsilon} \psi(x) dx$$

$$\left(\frac{d\psi(x)}{dx} \right)_{x=\varepsilon} - \left(\frac{d\psi(x)}{dx} \right)_{x=-\varepsilon} = -\frac{2m}{\hbar^2} V_0 \psi(0) = -2\alpha \psi(0) \quad (\text{boundary condition})$$

We use the parameter α as

$$\alpha = \frac{mV_0}{\hbar^2}.$$

The unit of α is [cm^{-1}]. Then the boundary condition is given by

$$(i) \quad \psi(+\varepsilon) = \psi(-\varepsilon)$$

$$(ii) \quad \left. \frac{d\psi(x)}{dx} \right|_{x=\varepsilon} - \left. \frac{d\psi(x)}{dx} \right|_{x=-\varepsilon} = -2\alpha \psi(0)$$

We assume that the energy E is negative (bound state). The Schrödinger equation is given by

$$\frac{d^2}{dx^2} \psi(x) = -\frac{2mE}{\hbar^2} \psi(x) = \rho^2 \psi(x)$$

where

$$\rho^2 = -\frac{2mE}{\hbar^2} (>0)$$

For $x < 0$, the solution for $\psi(x)$ is given by

$$\psi(x) = Ae^{\rho x}$$

For $x > 0$,

$$\psi(x) = Be^{-\rho x}$$

Since the potential energy $V(x)$ is an even function, the wave function should be either even or odd function. When the wave function is an odd function, the wave function should take a zero at the origin.

(i) The case when the wave function is an even function of x

$$A = B, \quad \rho = \alpha = \sqrt{-\frac{2mE}{\hbar^2}}$$

or

$$E = -\frac{\hbar^2}{2m}\alpha^2 = -\frac{mV_0^2}{2\hbar^2} \quad (\text{bound state}).$$

with

$$\alpha = \frac{mV_0}{\hbar^2}.$$

The unit of α is $[\text{cm}^{-2}]$.

From the normalization condition, we have

$$\psi(x) = \sqrt{\alpha} e^{-\alpha|x|}$$

(ii) The case when the wave function is an odd function of x

$$A = -B = 0.$$

So there is no trivial solution.

((Note)) Probability current density

The probability current density is defined by

$$j_x = \frac{1}{m} \operatorname{Re}[\psi^*(x) \frac{\hbar}{i} \frac{\partial}{\partial x} \psi(x)]$$

Suppose that the wave function is a real function of x . Then j_x should be equal to zero as shown above for the case of bound state case). In fact, the wave function is given by a real function.

2. Green's function: modified Helmholtz equation

We solve the problem (the bound state) using the Green function (see the APPENDIX). We start with the Schrodinger equation for the bound state

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) - V_0 \delta(x) \psi(x) = E \psi(x) = -\frac{\hbar^2 \rho^2}{2m} \psi(x)$$

where

$$E = -\frac{\hbar^2 \rho^2}{2m} (<0)$$

$$\left(\frac{d^2}{dx^2} - \rho^2\right) \psi(x) = L_x \psi(x) = -\frac{2m}{\hbar^2} V_0 \delta(x) \psi(x) = -f(x)$$

where

$$f(x) = \frac{2m}{\hbar^2} V_0 \delta(x) \psi(x) = 2\alpha \delta(x) \psi(x)$$

and

$$\alpha = \frac{mV_0}{\hbar^2}.$$

Using the 1D Green's function (modified Helmholtz), the solution of this equation can be given by

$$\begin{aligned}
\psi(x) &= \int G(x, \xi) f(\xi) d\xi \\
&= \int \frac{1}{2\rho} e^{-\rho|x-\xi|} 2\alpha\delta(\xi)\psi(\xi) d\xi \\
&= \frac{\alpha}{\rho} \psi(0) e^{-\rho|x|}
\end{aligned}$$

where

$$G(x, \xi) = \frac{1}{2\rho} e^{-\rho|x-\xi|} \quad (\text{Green's function: modified Helmholtz equation}).$$

At $x = 0$, we get

$$\psi(0) = \frac{\alpha}{\rho} \psi(0)$$

Then we have

$$\rho = \alpha, \quad E = -\frac{\hbar^2 \alpha^2}{2m}$$

The normalized wave function is

$$\psi(x) = \sqrt{\alpha} e^{-\alpha|x|}$$

3. Transmission of a "delta function" potential barrier for $E > 0$

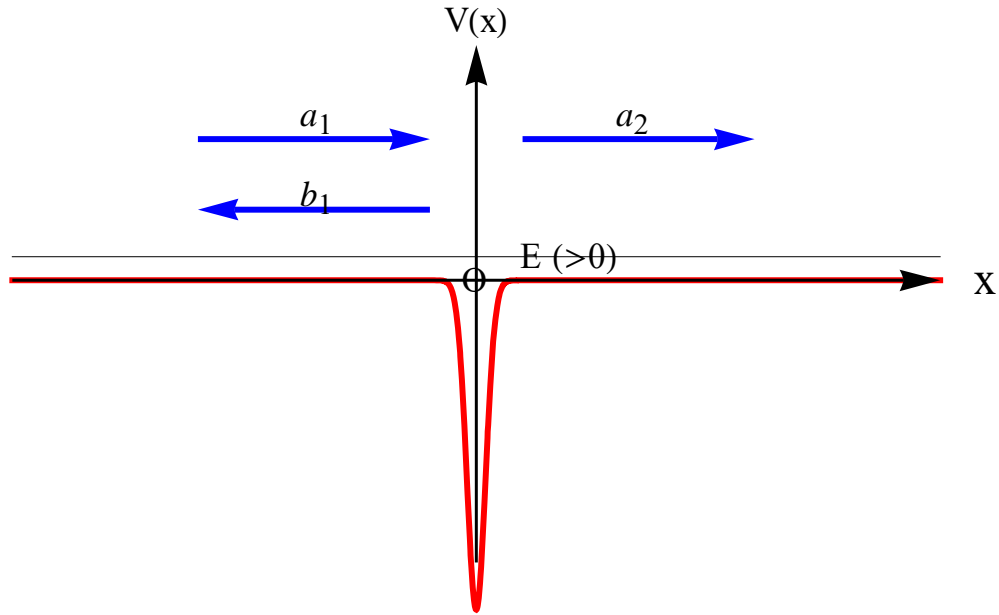


Fig. The transmission and reflection of free particle (with the positive energy E) in the presence of an attractive delta-function type potential.

For $x < 0$, we assume that

$$\psi_I = a_1 e^{ikx} + b_1 e^{-ikx}$$

where k is defined by

$$E = \frac{\hbar^2 k^2}{2m} (> 0)$$

The probability current density is

$$J_I = \frac{\hbar}{m} k (|a_1|^2 - |b_1|^2)$$

For $x > 0$, we assume that

$$\psi_{II} = a_2 e^{ikx}$$

The probability current density is

$$J_{II} = \frac{\hbar}{m} k |a_2|^2$$

From the continuity of the wave function at $x = 0$;

$$a_1 + b_1 = a_2 \quad (1)$$

From the condition

$$\left(\frac{d\psi(x)}{dx}\right)_{x=\varepsilon} - \left(\frac{d\psi(x)}{dx}\right)_{x=-\varepsilon} = -2\alpha\psi(0)$$

we get

$$ika_2 - ik(a_1 - b_1) = -2\beta a_2$$

or

$$a_1 - b_1 = \left(1 - i\frac{2\alpha}{k}\right)a_2, \quad (2)$$

Then we have

$$a_1 = \left(1 - i\frac{\alpha}{k}\right)a_2, \quad b_1 = i\frac{\alpha}{k}a_2$$

The transmissivity is

$$T = \frac{\frac{\hbar}{m} k |a_2|^2}{\frac{\hbar}{m} k |a_1|^2} = \frac{|a_2|^2}{|a_1|^2} = \frac{1}{1 + \frac{\alpha^2}{k^2}} = \frac{k^2}{\alpha^2 + k^2}$$

The reflectivity is

$$R = \frac{\frac{\hbar}{m} k |b_1|^2}{\frac{\hbar}{m} k |a_1|^2} = \frac{|b_1|^2}{|a_1|^2} = \frac{|a_2|^2}{|a_1|^2} \frac{|b_1|^2}{|a_2|^2} = \frac{\alpha^2}{\alpha^2 + k^2}.$$

where

$$T + R = 1.$$

The wave functions are obtained as

$$\begin{aligned}\psi_I &= a_1 e^{ikx} + b_1 e^{-ikx} \\ &= \left[\left(1 - i \frac{\alpha}{k}\right) e^{ikx} + i \frac{\alpha}{k} e^{-ikx} \right] a_2 R. \\ &= \left[e^{ikx} + \frac{2\alpha}{k} \sin(kx) \right] a_2\end{aligned}$$

$$\psi_{II} = a_2 e^{ikx}$$

where

$$\frac{\alpha}{k} = \frac{\frac{\sqrt{mV_0}}{\hbar}}{\frac{\sqrt{2mE}}{\hbar}} = \sqrt{\frac{V_0}{2E}}$$

((Mathematica))

We make a plot of the wave function in the regions I and II, where k and a are chosen appropriately.

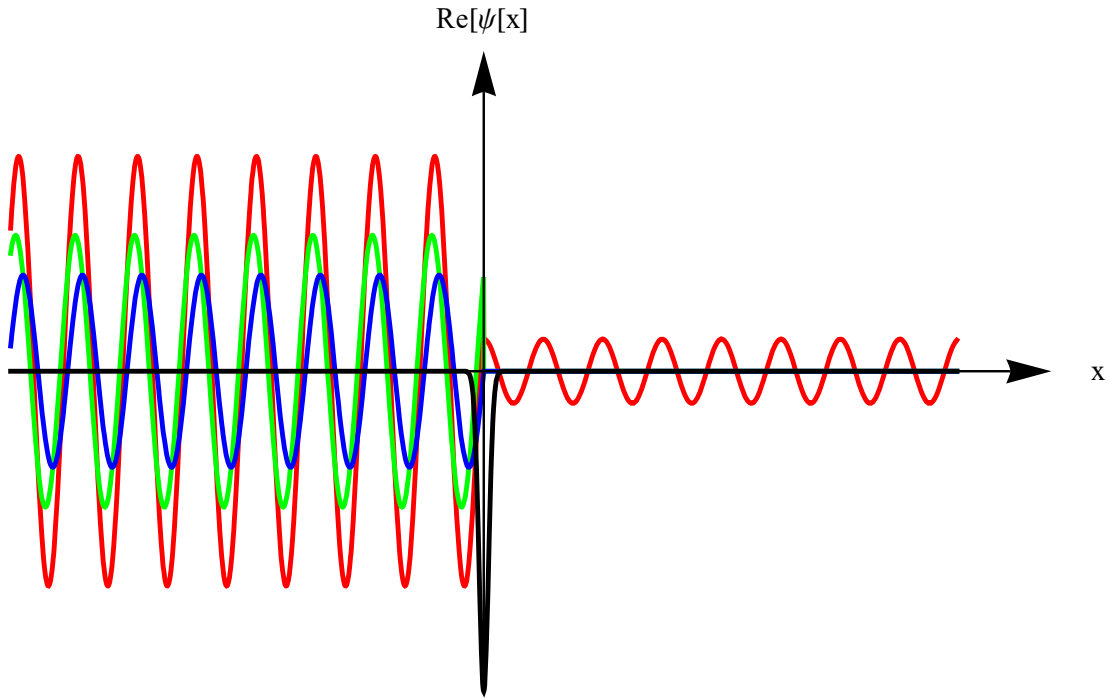
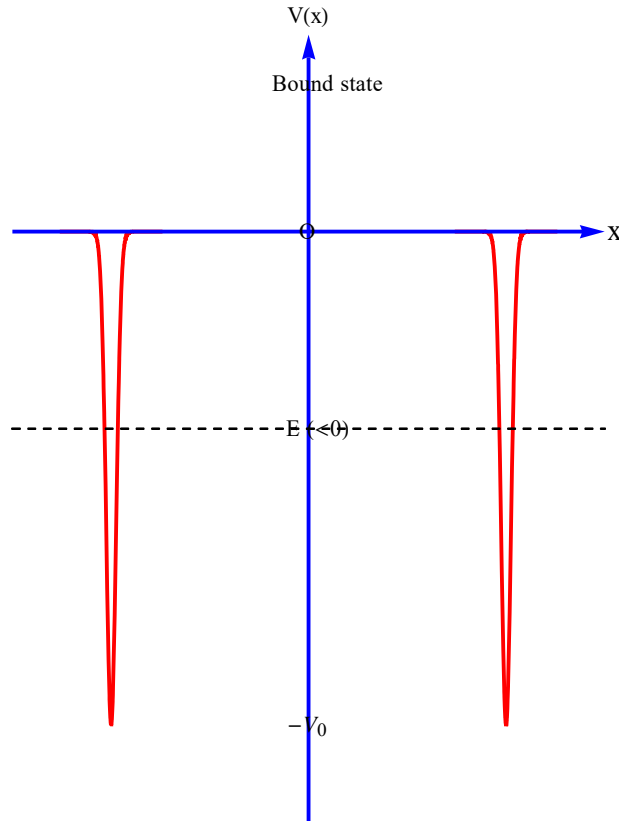


Fig. $k = 5$. $a = 5$. $|a_2| = 3$. Transmission and reflection of the free particle under the influence of a Dirac delta function type attractive potential (denoted by black). $f_{incident} = \text{Re}[a_1 e^{ikx}]$ (green, $x < 0$), $f_{reflected} = \text{Re}[b_1 e^{-ikx}]$ (blue, $x < 0$), $f_{total} = f_{incident} + f_{reflected}$ (red, $x < 0$), and $f_{transmitted} = \text{Re}[a_2 e^{ikx}]$ (red, $x > 0$)

4. Bound state under attractive double-delta potential

We discuss the eigenvalue (the bound state) problem for the Schrodinger equation for the attractive double-delta potential,



$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) - V_0 [\delta(x-a) + \delta(x+a)] \psi(x) = E \psi(x) = -\frac{\hbar^2 \rho^2}{2m} \psi(x)$$

where the potential energy is an even function of x ,

$$V(x) = V_0 [\delta(x-a) + \delta(x+a)]$$

and the energy is given by

$$E = -\frac{\hbar^2 \rho^2}{2m} (< 0)$$

for the bound state. Then we get

$$\left(\frac{d^2}{dx^2} - \rho^2\right) \psi(x) = L_x \psi(x) = -2\alpha [\delta(x-a) + \delta(x+a)] \psi(x) = -f(x)$$

where

$$\alpha = \frac{mV_0}{\hbar^2}.$$

Using the 1D Green's function (modified Helmholtz), the solution of this equation can be given by

$$\begin{aligned}\psi(x) &= \int G(x, \xi) f(\xi) d\xi \\ &= \int \frac{1}{2\rho} e^{-\rho|x-\xi|} 2\alpha[\delta(x-a) + \delta(x+a)] \psi(\xi) d\xi \\ &= \frac{\alpha}{\rho} [\psi(a)e^{-\rho|x-a|} + \psi(-a)e^{-\rho|x+a|}]\end{aligned}$$

where

$$L_x G(x, \xi) = -\delta(x - \xi)$$

$$\left(\frac{d^2}{dx^2} - \rho^2 \right) G(x, \xi) = -\delta(x - \xi)$$

↓

$$G(x, \xi) = \frac{1}{2\rho} e^{-\rho|x-\xi|} \quad (\text{Green's function: modified Helmholtz equation}).$$

At $x = a$

$$\psi(a) = \frac{\alpha}{\rho} [\psi(a) + \psi(-a)e^{-2\rho a}]$$

At $x = -a$

$$\psi(-a) = \frac{\alpha}{\rho} [\psi(a)e^{-2\rho a} + \psi(-a)]$$

We note that the wave function $\psi(x)$ is either an even function or an odd function of x .

(i) Even parity for the wave function

$$\psi_e(-a) = \psi_e(a)$$

or

$$1 = \frac{\alpha}{\rho} (e^{-2\rho a} + 1)$$

or

$$\frac{\rho}{\alpha} = 1 + e^{-2\rho a}$$

For simplicity we put

$$x = 2\rho a$$

$$\frac{x}{2a\alpha} = 1 + e^{-x}$$

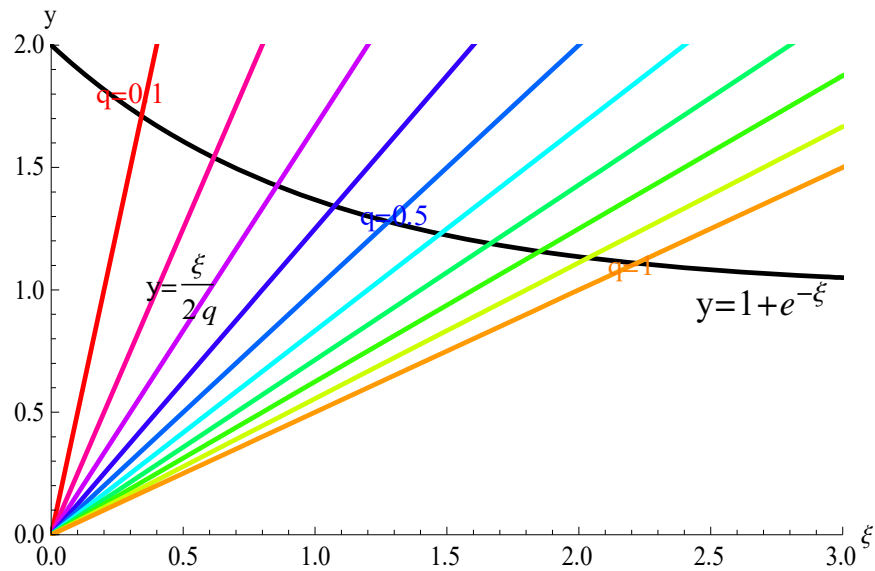


Fig. Even parity solution. Plot of $y = \frac{\xi}{2q}$ and $y = 1 + e^{-\xi}$ where q is changed as a parameter.

$\xi = 2\rho a$. $q = a\alpha$. The two curves intersect at a non-zero finite value of ξ . When $q = 1$, we have $\xi = 2.21772$. $y = 1.10886$.

The wave function (even parity) is given by

$$\frac{\psi_e(x)}{\psi_e(a)} = \frac{\alpha}{\rho} [e^{-\rho|x-a|} + e^{-\rho|x+a|}]$$

When $q = a\alpha = 1$, we have $x = 2\rho a = 2.21772$. For $a = 1$ and $\rho = 1.10886$, we make a plot of this function as a function of x . Clearly this function is an even function of x .

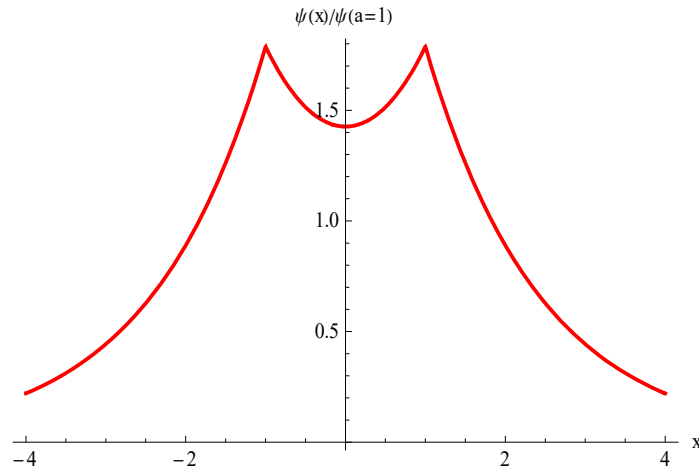


Fig. Plot of $\frac{\psi_e(x)}{\psi_e(a=1)}$ as a function of x . $\alpha = 1$. $a = 1$ and $\rho = 1.10886$.

(ii) Odd parity for the wave function

$$\psi_o(-a) = -\psi_o(a)$$

or

$$1 = \frac{\alpha}{\rho} (-e^{-2\rho a} + 1)$$

or

$$\frac{\rho}{\alpha} = -e^{-2\rho a} + 1$$

The value of ρ is obtained from the intersection of two curves

$$y = \frac{\xi}{2q}, \quad y = 1 - e^{-\xi}$$

with $\xi = 2\rho a$ and $q = a\alpha$ (parameter).

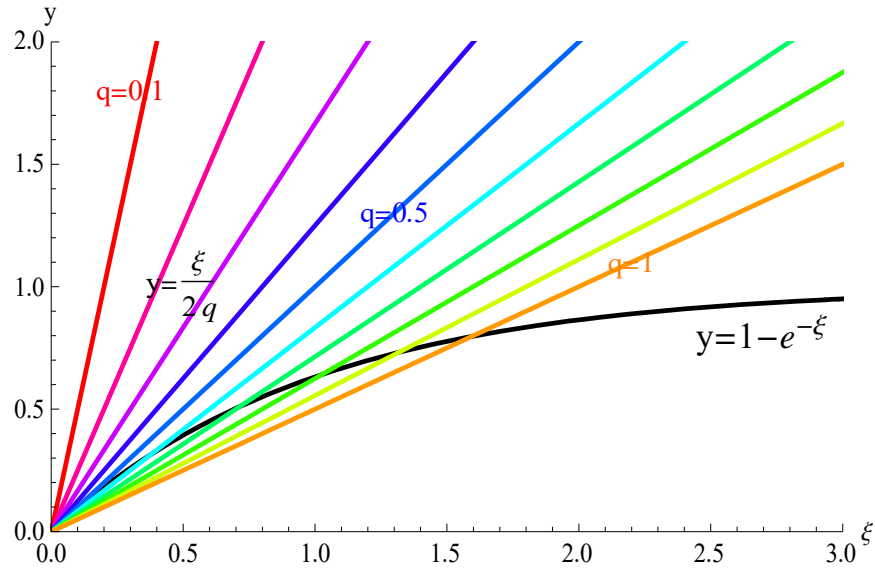


Fig. Odd parity solution. Plot of $y = \frac{\xi}{2q}$ and $y = 1 - e^{-\xi}$ where q is changed as a parameter.

$\xi = 2\rho a$. $q = a\alpha$. When $q > 0.5$, there are two solutions including $\xi = 0$. When $q < 0.5$, there is only one solution $\xi = 0$. When $q = 1$, we have $\xi = 1.59362$. $y = 0.796812$.

The wave function (odd parity) is given by

$$\frac{\psi_o(x)}{\psi_o(a)} = \frac{\alpha}{\rho} [e^{-\rho|x-a|} - e^{-\rho|x+a|}]$$

When $q = a\alpha = 1$, we have $\xi = 2\rho a = 1.59362$. For $a = 1$ and $\rho = 0.796812$, we make a plot of this function as a function of x . Clearly this function is an odd function of x .

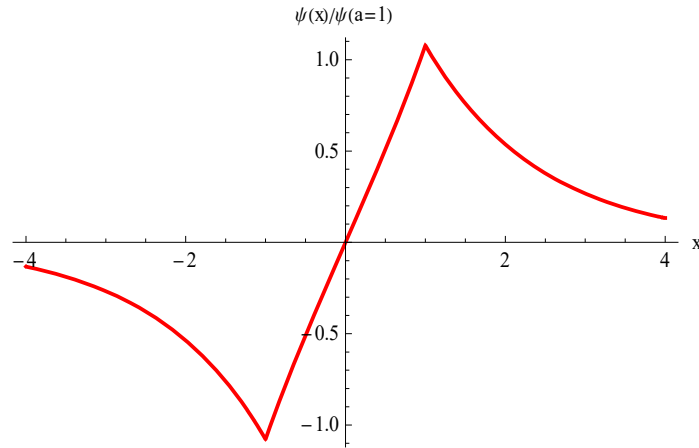


Fig. Plot of $\frac{\psi_o(x)}{\psi_o(a=1)}$ as a function of x . $\alpha = 1$. $a = 1$ and $\rho = 1.10886$.

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APPENDIX Green's function: modified Helmholtz equation

We construct the 1D Green's function for the modified Helmholtz equation

$$L_x \psi = \left(\frac{d^2}{dx^2} - k^2 \right) \psi .$$

Suppose that

$$L_x \psi = -f(x)$$

Using the Green's function we get

$$\psi = \int G(x, \xi) f(\xi) d\xi$$

$$L_x \psi = \int L_x G(x, \xi) f(\xi) d\xi = - \int \delta(x - \xi) f(\xi) d\xi = -f(x)$$

Thus we need $G(x, \xi)$ which satisfies

$$L_x G(x, \xi) = -\delta(x - \xi)$$

$$\left(\frac{d^2}{dx^2} - k^2 \right) G(x, \xi) = -\delta(x - \xi)$$

↓

$$G(x, \xi) = \frac{1}{2k} e^{-k|x-\xi|}$$

We consider the case at $\xi = 0$

$$\left(\frac{d^2}{dx^2} - k^2 \right) G(x) = -\delta(x)$$

$$G(q) = \frac{1}{\sqrt{2\pi}} \int G(x) e^{-iqx} dx$$

$$G(x) = \frac{1}{\sqrt{2\pi}} \int G(q) e^{iqx} dq$$

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{iqx} dq$$

$$\frac{1}{\sqrt{2\pi}} \int \left(\frac{d^2}{dx^2} - k^2 \right) G(q) e^{iqx} dq = -\frac{1}{2\pi} \int e^{iqx} dq$$

or

$$\frac{1}{\sqrt{2\pi}} \int (-q^2 - k^2) G(q) e^{iqx} dq = -\frac{1}{2\pi} \int e^{iqx} dq.$$

Then we have

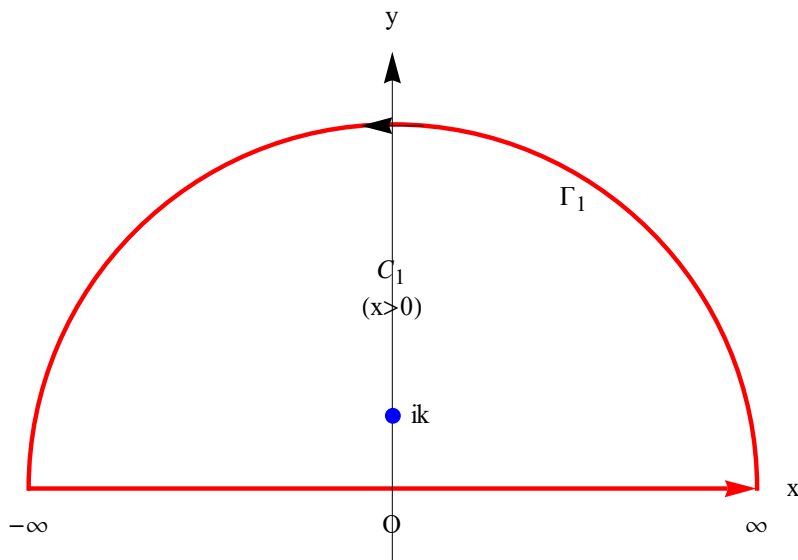
$$(-q^2 - k^2)G(q) = -\frac{1}{\sqrt{2\pi}} \quad \text{or} \quad G(q) = \frac{1}{\sqrt{2\pi}} \frac{1}{q^2 + k^2}$$

$$G(x) = \frac{1}{2\pi} \int \frac{e^{iqx}}{q^2 + k^2} dq$$

(i) For $x > 0$

$$G(x) = \frac{1}{2\pi} \int_{C_1} \frac{e^{iqx}}{q^2 + k^2} dq = \frac{1}{2k} e^{-kx}$$

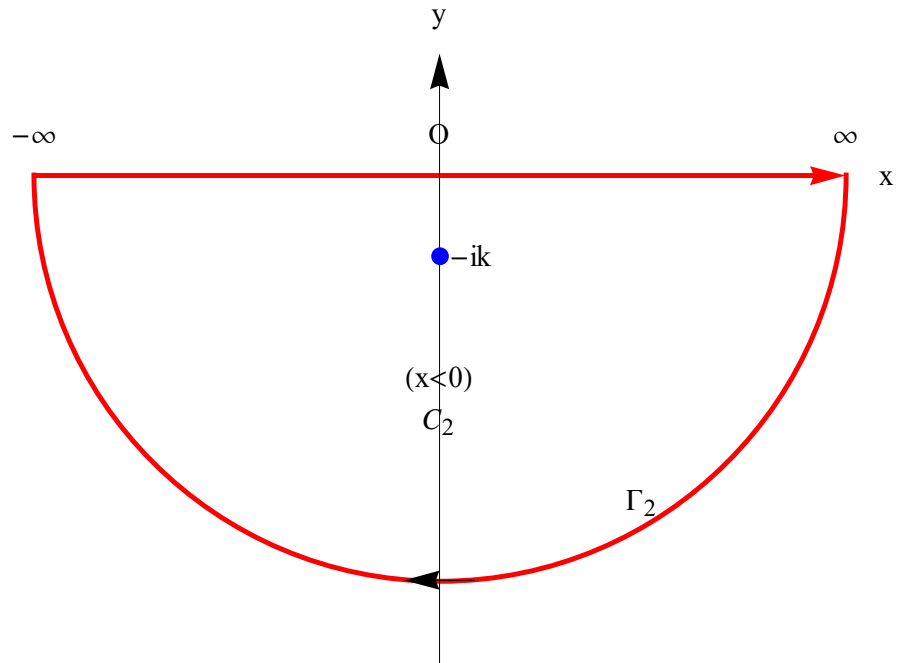
where C_1 is in the lower-half plane (counter-clock wise). There is a simple pole of $z = i k$ inside the contour C_1 . We use the Residue theorem.



(ii) For $x < 0$

$$G(x) = \frac{1}{2\pi} \int_{C_2} \frac{e^{iqx}}{q^2 + k^2} dq = \frac{1}{2k} e^{kx}$$

where C_2 is in the lower-half plane (clock-wise). There is a simple pole of $z = -i k$ inside the contour C_2 . We use the residue theorem.



In summary we have the Green's function

$$G(x) = \frac{1}{2k} e^{-k|x|}$$

or

$$G(x, \xi) = \frac{1}{2k} e^{-k|x-\xi|}$$