

运行说明

推导本征能量方程

由于V为偶函数, 不失一般性可假设波函数解为奇函数或偶函数, 波函数解形式如下:

$$\begin{aligned}\text{偶数能级 } u(x) &= \begin{cases} Be^{kx}, & x < -a \\ A\cos qx, & -a < x < a \\ Be^{-kx}, & x > a \end{cases} \\ \text{奇数能级 } u(x) &= \begin{cases} De^{kx}, & x < -a \\ C\sin qx, & -a < x < a \\ -De^{-kx}, & x > a \end{cases}\end{aligned}$$

无量纲化 $\kappa = ka, \xi = \frac{x}{a}, \theta = qa$. 由于奇偶性, 仅需考虑势阱一侧波函数的连续性.

偶数能级

$$\begin{aligned}u(\xi) &= \begin{cases} Be^{\kappa\xi}, & \xi < -1 \\ A\cos\theta\xi, & -1 < \xi < 1 \\ Be^{-\kappa\xi}, & \xi > 1 \end{cases} \\ u'(\xi) &= \begin{cases} B\kappa e^{\kappa\xi}, & \xi < -1 \\ -A\theta\sin\theta\xi, & -1 < \xi < 1 \\ -B\kappa e^{-\kappa\xi}, & \xi > 1 \end{cases}\end{aligned}$$

$$u(-1_-) = u(-1_+) \text{ 得 } Be^{-\kappa} = A\cos\theta$$

$$u'(-1_-) = u'(-1_+) \text{ 得 } B\kappa e^{-\kappa} = A\theta\sin(\theta)$$

$$\text{故 } \kappa = \theta \tan(\theta), \text{ 即 } \sqrt{\frac{|E|}{V_0 - |E|}} = \tan \frac{\sqrt{2m(V_0 - |E|)}a}{\hbar}$$

奇数能级

$$\begin{aligned}u(\xi) &= \begin{cases} De^{\kappa\xi}, & \xi < -1 \\ C\sin\theta\xi, & -1 < \xi < 1 \\ -De^{-\kappa\xi}, & \xi > 1 \end{cases} \\ u'(\xi) &= \begin{cases} D\kappa e^{\kappa\xi}, & \xi < -1 \\ C\theta\cos\theta\xi, & -1 < \xi < 1 \\ D\kappa e^{-\kappa\xi}, & \xi > 1 \end{cases}\end{aligned}$$

$$u(-1_-) = u(-1_+) \text{ 得 } De^{-\kappa} = -C\sin\theta$$

$$u'(-1_-) = u'(-1_+) \text{ 得 } D\kappa e^{-\kappa} = C\theta\cos(\theta)$$

$$\text{故 } -\theta \cot(\theta) = \kappa, \text{ 即 } -\sqrt{\frac{|E|}{V_0 - |E|}} = \cot \frac{\sqrt{2m(V_0 - |E|)}a}{\hbar}$$

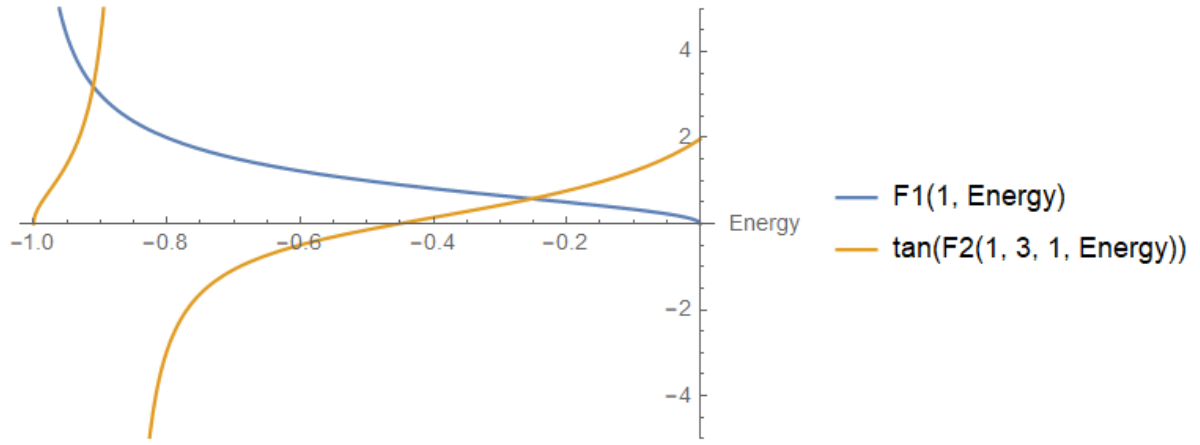
代入参数, 使用Mathematica对偶数和奇数能级的本征能量方程作图. 由于已选用自然单位制, 可略去 \hbar .

由于粒子处于束缚态, 有 $E < 0$, 故 $|E| = -E$, 两个方程化为:

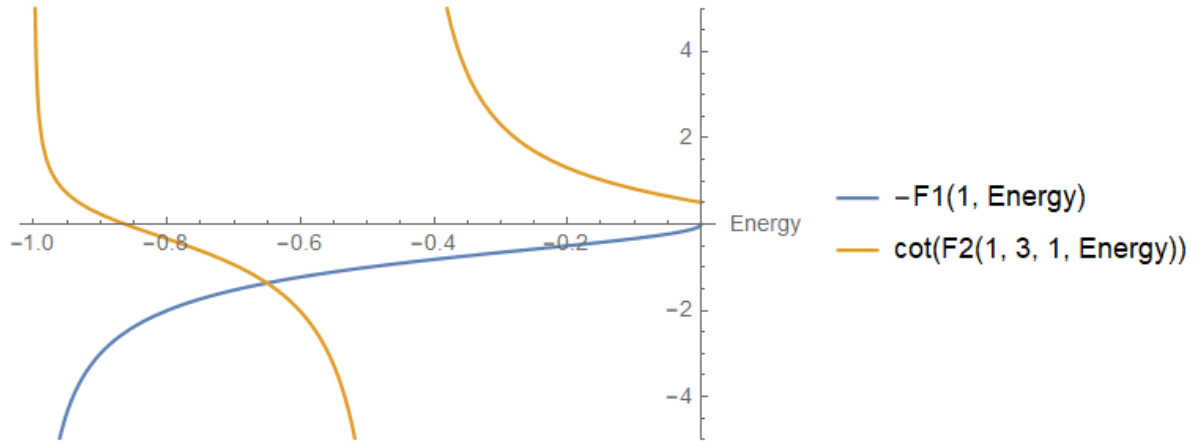
$$\begin{aligned}\sqrt{\frac{-E}{V_0 + E}} &= \tan \frac{\sqrt{2m(V_0 + E)}a}{\hbar} \\ -\sqrt{\frac{-E}{V_0 + E}} &= \cot \frac{\sqrt{2m(V_0 + E)}a}{\hbar}\end{aligned}$$

作图得:

偶数能级:



奇数能级:



故该系统本征能量共有三个解. 使用数值解法求出三个本征能量为:

$$\text{偶数能级: } E1 = -0.911\text{GeV}, E3 = -0.253\text{GeV}$$

$$\text{奇数能级: } E2 = -0.650\text{GeV}$$

代入方程并利用归一化条件求解系数, 得波函数表达式并作图.

$$\text{对于偶数能级, } A = \frac{Be^{-\kappa}}{\cos\theta}$$

$$\text{定义 } u_{\text{even}}(\xi) = \begin{cases} e^{\kappa\xi}, & \xi < -1 \\ \frac{e^{-\kappa}}{\cos\theta} \cos(\theta\xi), & -1 < \xi < 1 \\ e^{-\kappa\xi}, & \xi > 1 \end{cases}$$

$$\text{归一化: } I_{\text{even}} = \int_{-\infty}^{\infty} u_{\text{even}}(\xi) d\xi$$

$$\text{则 } B = \sqrt{1/I_{\text{even}}}$$

$$\text{对于奇数能级, } C = \frac{-De^{-\kappa}}{\sin\theta}$$

$$\text{定义 } u_{\text{odd}}(\xi) = \begin{cases} e^{\kappa\xi}, & \xi < -1 \\ \frac{-e^{-\kappa}}{\sin\theta} \sin(\theta\xi), & -1 < \xi < 1 \\ -e^{-\kappa\xi}, & \xi > 1 \end{cases}$$

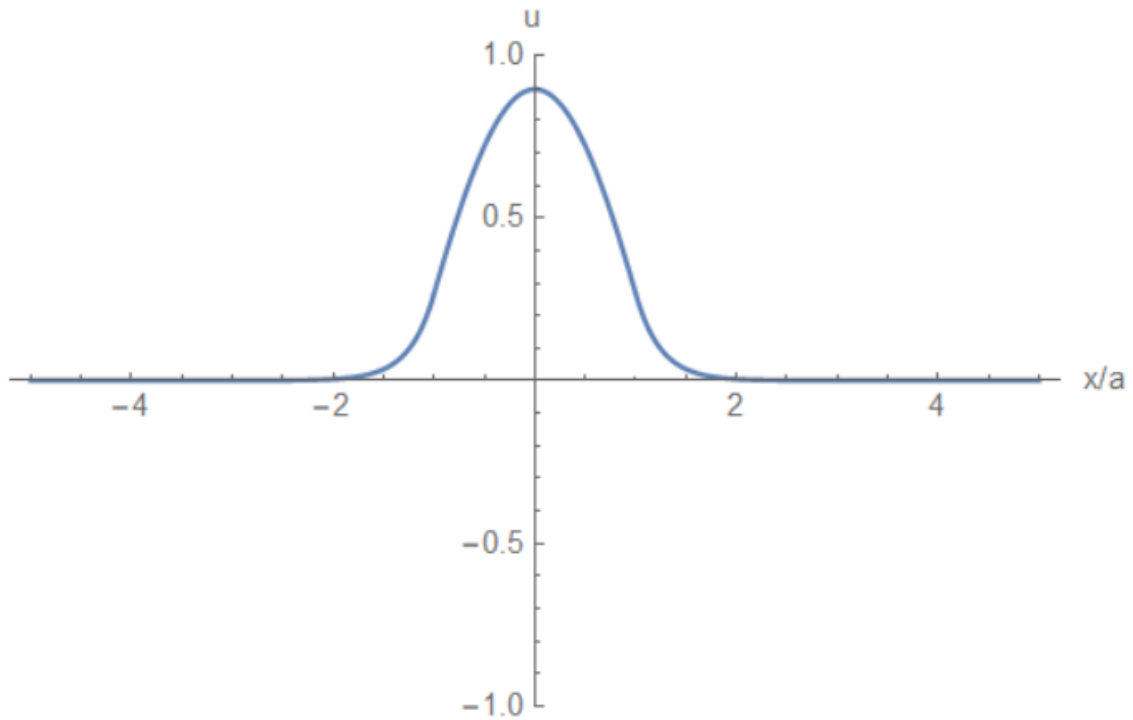
$$\text{归一化: } I_{\text{odd}} = \int_{-\infty}^{\infty} u_{\text{odd}}(\xi) d\xi$$

$$\text{则 } D = \sqrt{1/I_{\text{odd}}k}$$

使用 $\xi = x/a$ 无量纲化, 有:

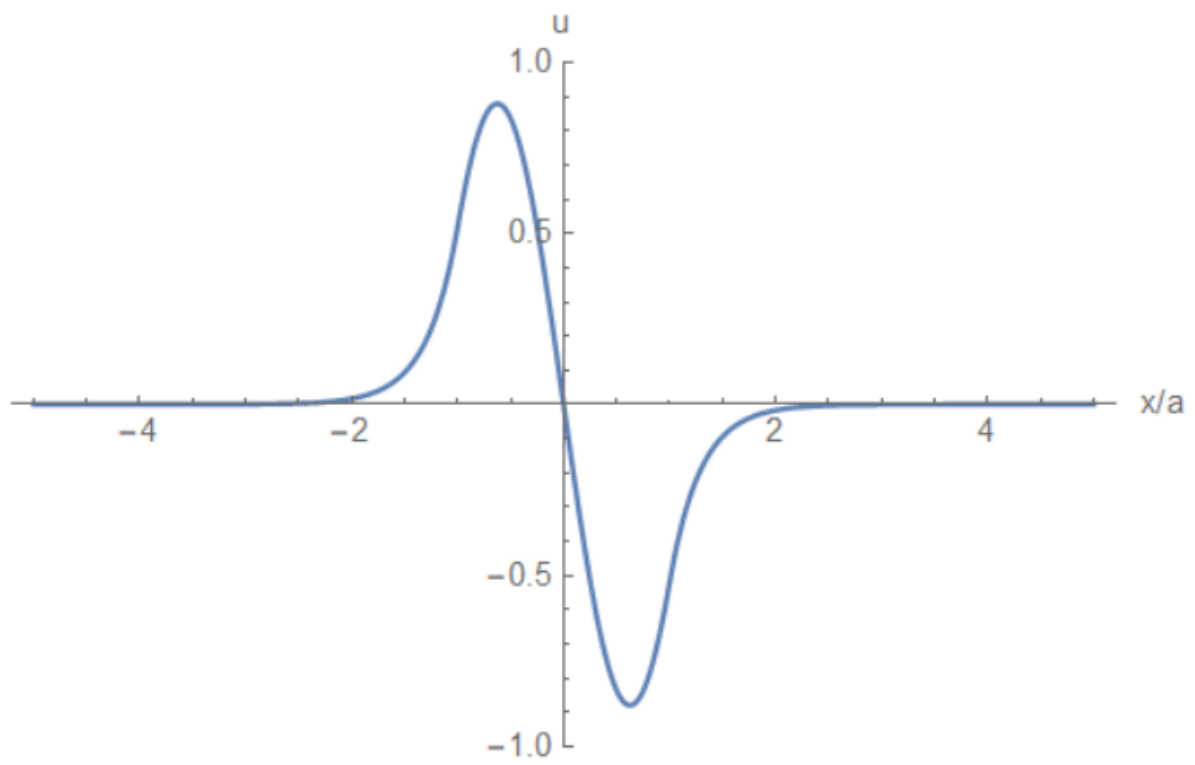
$E1 = -0.911 GeV$ 时, $u_1(x) =$

$$\left[\begin{array}{ll} 0.267521 \times 2.71828^{4.0489 + 4.0489 \xi} & \xi < -1. \\ 0.895509 \cos [1.26743 \xi] & -1. < \xi < 1. \\ 0.267521 \times 2.71828^{4.0489 - 4.0489 \xi} & \xi > 1. \\ 0. & \text{True} \end{array} \right.$$



$E2 = -0.650 GeV$ 时, $u_2(x) =$

$$\left[\begin{array}{ll} 2.71828^{3.42134 \xi} & \xi < -1. \\ -0.0552444 \sin [2.50887 \xi] & -1. < \xi < 1. \\ -1. \times 2.71828^{-3.42134 \xi} & \xi > 1. \\ 0. & \text{True} \end{array} \right.$$



$E_3 = -0.253 \text{ GeV}$ 时, $u_3(x) =$

$$\left\{ \begin{array}{ll} 0.520191 \times 2.71828^{3.42134 + 3.42134 \xi} & \xi < -1. \\ -0.879673 \sin[2.50887 \xi] & -1. < \xi < 1. \\ -0.520191 \times 2.71828^{3.42134 - 3.42134 \xi} & \xi > 1. \\ 0. & \text{True} \end{array} \right.$$

