Chapter 3: The WKB Approximation

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1 Introduction

薛定谔方程

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x) + \frac{2m}{\hbar^2}\left[E - V(x)\right]\psi(x) = 0 \tag{1}$$

令

$$k^2(x) = \frac{2m}{\hbar^2}\left[E - V(x)\right] \tag{2}$$

薛定谔方程可以写成

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x) + k^2(x)\psi(x) = 0 \tag{3}$$

这是 Sturm-Liouville 方程，是最普遍的二阶微分方程。

当 $V(x) = V$ 时，

$$\psi(x) = Ae^{\pm ikx} \tag{4}$$

受此启发，做近似

$$\psi(x) = A\exp\left[\pm i\int^x k(x')\mathrm{d}x'\right] \tag{5}$$

什么时候是好的近似呢？当然是当 $V(x)$ 变化慢的时候，但 $V(x)$ 变化快慢用什么来定义？我们应该把它定量化，接下来解决这一个问题。

$$\psi'(x) = A\exp\left[\pm i\int^x k(x')\mathrm{d}x'\right]\left[\pm ik(x)\right] \tag{6}$$

$$\psi''(x) = A\exp\left[\pm i\int^x k(x')\mathrm{d}x'\right]\left[-k^2(x)\right] + A\exp\left[\pm i\int^x k(x')\mathrm{d}x'\right]\left[\pm ik'(x)\right] \tag{7}$$

代入薛定谔方程，得到

$$\left[-k^2(x) \pm ik'(x) + k^2(x)\right]\psi(x) = 0 \tag{8}$$

上式在什么情况下成立呢?

$$-k^2(x) \pm ik'(x) + k^2(x) = 0 \tag{9}$$

即

$$\left|\frac{k'(x)}{k^2(x)}\right| \ll 1 \tag{10}$$

$$2k(x)k'(x) = \frac{4m}{\hbar^2}\cdot\left[E - V(x)\right]^{\frac{1}{2}}\cdot\frac{1}{2}\left[E - V(x)\right]^{-\frac{1}{2}}\left[-V'(x)\right] = -\frac{2m}{\hbar^2}V'(x) \tag{11}$$

$$\left|\frac{m}{\hbar^2}\frac{V'(X)}{k^3(x)}\right| \ll 1 \tag{12}$$

即

$$\left|\frac{mV'(X)}{\{2m[E-V(x)]\}^{\frac{3}{2}}}\right|\hbar \ll 1 \tag{13}$$

- 当 $\hbar \to 0$ 时，为半经典近似，能够很好地满足上述不等式。
- 当 $V'(x)$ 很小，即势能变化缓慢时，能够很好地满足上述不等式。
- 当 $E = V(x)$ 时，是经典和量子的拐点 (dangerous point)，近似可能失败。

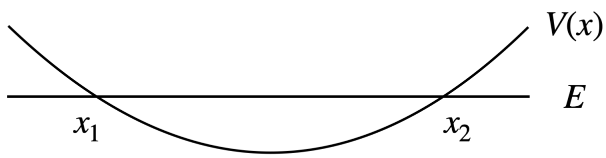
得到好的近似的条件后，我们继续解薛定谔方程

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x) + \frac{2m}{\hbar^2}\left[E - V(x)\right]\psi(x) = 0 \tag{14}$$

$$k^2(x) = \frac{2m}{\hbar^2}\left[E - V(x)\right] \tag{15}$$

近似解

$$\psi(x) = A\exp\left[\pm i\int^x k(x')\mathrm{d}x'\right] \tag{16}$$



当 $x > x_1$ 时，

$$\begin{aligned}\psi(x) &= A_1\exp\left[i\int_{x_1}^x k(x')\mathrm{d}x'\right] + A_2\exp\left[-i\int_{x_1}^x k(x')\mathrm{d}x'\right] \\ &\sim \cos\left[\int_{x_1}^x k(x')\mathrm{d}x' + \eta_1\right]\end{aligned} \tag{17}$$

当 $x < x_2$ 时

$$\begin{aligned}\psi(x) &= A_1^{'}\exp\left[i\int_{x_2}^x k(x')\mathrm{d}x'\right] + A_2^{'}\exp\left[-i\int_{x_2}^x k(x')\mathrm{d}x'\right] \\ &\sim \cos\left[\int_{x_2}^x k(x')\mathrm{d}x' - \eta_2\right] \\ &= \cos\left[\int_{x_1}^x k(x')\mathrm{d}x' + \int_{x_2}^{x_1} k(x')\mathrm{d}x' - \eta_2\right]\end{aligned} \tag{18}$$

这两个解本质上是同一个解，比较两解

$$\int_{x_2}^{x_1} k(x')\mathrm{d}x' - \eta_2 = n\pi + \eta_1 \tag{19}$$

$$\int_{x_1}^{x_2} k(x')\mathrm{d}x' = n\pi - (\eta_1 + \eta_2) \qquad n = 0, \pm 1, \pm 2, \cdots \tag{20}$$

$$k(x) \sim \sqrt{E - V(x)} \tag{21}$$

由此 Eq.(20) 给出了能量的条件，并显示出能量是分立的，即给出能量的量子化条件。

目前 η_1 和 η_2 仍为未知量，我们需要让近似更进一步。

2 Approximation Including the Next Order

为了得到更精确的解，我们将近似解写成

$$\psi(x) = A(x)\exp\left[\pm i\int^x k(x')\mathrm{d}x'\right] \tag{22}$$

接下来我们要做的是确定 $A(x)$。

$$\psi'(x) = A'(x)\exp\left[\pm i\int^x k(x')\mathrm{d}x'\right] + A(x)\exp\left[\pm i\int^x k(x')\mathrm{d}x'\right][\pm ik(x)] \tag{23}$$

$$\begin{aligned}\psi''(x) =& A''(x)\exp\left[\pm i\int^x k(x')\mathrm{d}x'\right] + A'(x)\exp\left[\pm i\int^x k(x')\mathrm{d}x'\right][\pm ik(x)] \\ &+ A'(x)\exp\left[\pm i\int^x k(x')\mathrm{d}x'\right][\pm ik(x)] + A(x)\exp\left[\pm i\int^x k(x')\mathrm{d}x'\right]\left[-k^2(x)\right] \\ &+ A(x)\exp\left[\pm i\int^x k(x')\mathrm{d}x'\right][\pm ik'(x)] \\ =& A''(x)\exp\left[\pm i\int^x k(x')\mathrm{d}x'\right] + 2A'(x)\exp\left[\pm i\int^x k(x')\mathrm{d}x'\right][\pm ik(x)] \\ &+ A(x)\exp\left[\pm i\int^x k(x')\mathrm{d}x'\right]\left[-k^2(x)\right] + A(x)\exp\left[\pm i\int^x k(x')\mathrm{d}x'\right][\pm ik'(x)] \\ =& -k^2(x)A(x)\exp\left[\pm i\int^x k(x')\mathrm{d}x'\right]\end{aligned} \tag{24}$$

即

$$A''(x) + 2A'(x)[\pm ik(x)] + A(x)[\pm ik'(x)] = 0 \tag{25}$$

近似确定 $A(x)$，忽略 $A'(x)$

$$2A'(x)k(x) = -A(x)k'(x) \tag{26}$$

$$\frac{A'(x)}{A(x)} = -\frac{1}{2}\frac{k'(x)}{k(x)} \tag{27}$$

$$\int\frac{A'(x)}{A(x)}\mathrm{d}x = -\frac{1}{2}\int\frac{k'(x)}{k(x)}\mathrm{d}x \tag{28}$$

$$\ln A(x) = -\frac{1}{2}\ln k(x) + \tilde{A} \tag{29}$$

$$A(x) = |k(x)|^{-\frac{1}{2}}\tilde{A} \tag{30}$$

代入 $\psi(x)$ 近似解得

$$\psi(x) = \tilde{A}|k(x)|^{-\frac{1}{2}}\exp\left[\pm i\int^x k(x')\mathrm{d}x'\right] \tag{31}$$

当 $E = V(x)$ 即当 $k(x) = 0$ 时，$\psi(x)$ 趋于无穷大，因此进一步近似仍然不够。

3 Semiclassical Expansion

$$\psi(x) = A\exp\left[\frac{i}{\hbar}S(x)\right] \tag{32}$$

$$\psi'(x) = A\exp\left[\frac{i}{\hbar}S(x)\right]\frac{i}{\hbar}S'(x) \tag{33}$$

$$\psi''(x) = A\exp\left[\frac{i}{\hbar}S(x)\right]\left[-\frac{1}{\hbar^2}S'^2(x)\right] + A\exp\left[\frac{i}{\hbar}S(x)\right]\frac{i}{\hbar}S''(x) \tag{34}$$

代入薛定谔方程，得

$$\frac{i}{\hbar}S''(x) - \frac{1}{\hbar^2}S'^2(x) + k^2(x) = 0 \tag{35}$$

即

$$i\hbar S''(x) - S'^2(x) + 2m[E - V(x)] = 0 \tag{36}$$

由此可知 $S(x,\hbar)$。当 $\hbar \to 0$ 时退化为经典理论。设 $\hbar$ 是小量，用 $\hbar$ 做泰勒展开

$$S(x) = S_0(x) + \hbar S_1(x) + \hbar^2 S_2(x) + \cdots = \sum_{n=0}^{\infty}\hbar^n S_n(x) \tag{37}$$

代入薛定谔方程

$$i\hbar[S_0''(x) + \hbar S_1''(x) + \hbar^2 S_2''(x)] - [S_0'(x) + \hbar S_1'(x) + \hbar^2 S_2'(x)]^2 + 2m[E - V(x)] = 0 \tag{38}$$

分别比较 h^0, h^1, h^2 的系数

$$-S_0'^2 + 2m[E - V(x)] = 0 \tag{39}$$

$$iS_0''(x) - 2S_0'(x)S_1'(x) = 0 \tag{40}$$

得到

$$S_0'(x) = \pm\hbar k(x) \tag{41}$$

$$S_0(x) = \pm\hbar\int_{x_0}^{x} k(x')\mathrm{d}x' \tag{42}$$

$$\psi(x) = A\exp\left[\frac{i}{\hbar}S_0(x)\right] = A\exp\left[\pm i\int_{x_0}^{x} k(x')\mathrm{d}x'\right] \tag{43}$$

又 Eq.(40)

$$\frac{iS_0''(x)}{2S_0'(x)} = s_1'(x) \tag{44}$$

解得

$$S_1(x) = \frac{i}{2}\ln|k(x)| \tag{45}$$

$$\begin{aligned}\psi(x) &= A\exp\left\{\frac{i}{\hbar}[S_0(x) + \hbar S_1(x)]\right\} = A\exp\left\{\frac{i}{\hbar}\left[\pm\hbar\int_{x_0}^{x} k(x')\mathrm{d}x' + \hbar\frac{i}{2}\ln|k(x)|\right]\right\} \\ &= A\exp\left[\pm i\int_{x_0}^{x} k(x')\mathrm{d}x' - \frac{1}{2}\ln|k(x)|\right] = A|k(x)|^{-\frac{1}{2}}\exp\left[\pm i\int_{x_0}^{x} k(x')\mathrm{d}x'\right]\end{aligned} \tag{46}$$

用 $\hbar$ 做半经典系统展开是物理学家做的事情，而解微分方程不仅是物理学家做的事情，数学家做得更早，接下来我们讨论数学家在解微分方程上做的工作。

4 Mathematician's Work

WKB(Wentzel–Kramers–Brillouin) 近似又叫 WKBJ 近似，其中"J"代表 Harold Jeffreys。1923 年 Jeffreys 发展出一种近似解线性二阶微分方程解的一般方法，这一类方程包括薛定谔方程。而薛定谔方程本身是在两年后才发展起来的。

$$\frac{\mathrm{d}}{\mathrm{d}x}\left[p(x)\frac{\mathrm{d}y}{\mathrm{d}x}\right] + [\lambda^2 q_0(x) + q_1(x)]y = 0 \tag{47}$$

这是最典型的二阶线性微分方程——Sturm-Liouville 方程。薛定谔方程是 Sturm-Liouville 方程的特殊情况(当 $p(x)$ 和 $q_1(x)$ 是常数时)。1837 年 Liouville 指出 Sturm-Liouville 方程总能化成薛定谔方程的形式。

引入变量

$$t = \int_{x_0}^{x} \left[\frac{q_0(x')}{p(x')}\right]^{\frac{1}{2}} \mathrm{d}x' \tag{48}$$

$$w(x) = [q_0(x)p(x)]^{\frac{1}{4}}\, y(x) \tag{49}$$

Sturm-Liouville 方程化为

$$\frac{\mathrm{d}^2 w}{\mathrm{d}t^2} + \lambda^2 w = \left[(q_0 p)^{-\frac{1}{4}} \frac{\mathrm{d}^2}{\mathrm{d}t^2}(q_0 p)^{\frac{1}{4}} - \frac{q_1}{q_0}\right] w \tag{50}$$

令

$$r(t) = (q_0 p)^{-\frac{1}{4}} \frac{\mathrm{d}^2}{\mathrm{d}t^2}(q_0 p)^{\frac{1}{4}} - \frac{q_1}{q_0} \tag{51}$$

则

$$\frac{\mathrm{d}^2 w}{\mathrm{d}t^2} + \lambda^2 w = r(t) w \tag{52}$$

在 Feynman 路径积分中我们已经知道，这类微分方程总可以写成积分方程的形式

$$w(t) = c_1 \cos\lambda t + c_2 \sin\lambda t + \int_{t_0}^{t} \frac{\sin\lambda(t-s)}{\lambda} r(s) w(s) \mathrm{d}s \tag{53}$$

代入 Eq.(52) 即可验证。

对于薛定谔方程

$$\lambda^2 q_0(x) = \frac{2m}{\hbar^2}[E - V(x)] \qquad p(x) = 1 \tag{54}$$

$\lambda \to 0$ 对应 $\hbar \to 0$ 即半经典近似。当 $\lambda \to \infty$ 时

$$|c_1 \cos\lambda t + c_2 \sin\lambda t| \gg \left|\int_{t_0}^{t} \frac{\sin\lambda(t-s)}{\lambda} r(s) w(s) \mathrm{d}s\right| \tag{55}$$

零级近似

$$w(t) = c_1 \cos\lambda t + c_2 \sin\lambda t \tag{56}$$

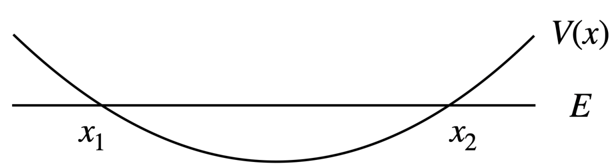
将

$$t = \int_{x_0}^{x} \left[\frac{q_0(x')}{p(x')}\right]^{\frac{1}{2}} \mathrm{d}x' \tag{57}$$

代入 $w(t)$，则

$$\begin{aligned} y(x) &= [q_0(x)p(x)]^{-\frac{1}{4}}\, w(x) \\ &= [q_0 p]^{-\frac{1}{4}} \left\{ c_1 \cos\left[\lambda \int_{x_0}^{x} \left(\frac{q_0}{p}\right)^{\frac{1}{2}} \mathrm{d}x'\right] + c_2 \sin\left[\lambda \int_{x_0}^{x} \left(\frac{q_0}{p}\right)^{\frac{1}{2}} \mathrm{d}x'\right] \right\} \\ &= \sqrt{\frac{\lambda}{k(x)}} \left\{ c_1 \cos\left[\int_{x_0}^{x} k(x') \mathrm{d}x'\right] + c_2 \sin\left[\int_{x_0}^{x} k(x') \mathrm{d}x'\right] \right\} \end{aligned} \tag{58}$$

5 Bound States



当 $x > x_1$ 时

$$\psi(x) \sim \cos\left(\int_{x_1}^{x} k(x')\mathrm{d}x' + \eta_1\right) \tag{59}$$

当 $x < x_2$ 时

$$\psi(x) \sim \cos\left(\int_{x_2}^{x} k(x')\mathrm{d}x' - \eta_2\right) \tag{60}$$

$$\int_{x_1}^{x_2} k(x)\mathrm{d}x = n\pi - (\eta_1 + \eta_2) \tag{61}$$

给出了能量的量子化条件，其本质上是微分方程的性质。接下来我们来确定 η_1 和 η_2。

首先定义

$$\kappa(x) = \begin{cases} \frac{1}{\hbar}\sqrt{2m[V(x)-E]} & V(x) > E \\ \frac{1}{\hbar}\sqrt{2m[E-V(x)]} & V(x) < E \end{cases} \tag{62}$$

从 x_1 的方向看，当 $x < x_1$ 时，

$$\psi(x) = A\frac{1}{[\kappa(x)]^{\frac{1}{2}}}\exp\left[-\int_{x}^{x_1}\kappa(x')\mathrm{d}x'\right] \tag{63}$$

当 $x > x_1$ 时，

$$\psi(x) = B\frac{1}{[\kappa(x)]^{\frac{1}{2}}}\cos\left[\int_{x_1}^{x}\kappa(x')\mathrm{d}x' + \tilde{\eta}_1\right] \tag{64}$$

当 $x = x_1$ 时，$\kappa(x) = 0$，此时波函数的解变为无穷大，而这显然不成立。接下来我们来近似求当 $x = x_1$ 时的严格解。当 $x \to x_1$ 时，做线性展开

$$E - V(x) = -\left.\frac{\mathrm{d}V(x)}{\mathrm{d}x}\right|_{x_1}(x - x_1) \tag{65}$$

代入薛定谔方程

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x) + V(x)\psi(x) = E\psi(x) \tag{66}$$

令

$$\xi = \left(-\frac{2m}{\hbar^2}\left.\frac{\mathrm{d}V(x)}{\mathrm{d}x}\right|_{x_1}\right)^{\frac{1}{3}}(x - x_1) \tag{67}$$

其中 ξ 和 $(x - x_1)$ 同号。薛定谔方程可化为 Airy equation

$$\frac{\mathrm{d}^2}{\mathrm{d}\xi^2}\psi + \xi\psi = 0 \tag{68}$$

它的解

$$\psi \sim \frac{1}{\sqrt{\pi}}\int_0^\infty \cos\left(\frac{1}{3}u^3 - u\xi\right)\mathrm{d}u \tag{69}$$

查数学用表可知解的渐进行为。当 $\xi \to -\infty$ 时，

$$\psi \sim \frac{A}{|\xi|^{\frac{1}{4}}}\exp\left(-\frac{2}{3}|\xi|^{\frac{3}{2}}\right) \tag{70}$$

当 $\xi \to \infty$ 时，

$$\psi \sim \frac{B}{\xi^{\frac{1}{4}}}\cos\left(\frac{2}{3}\xi^{\frac{3}{2}} - \frac{1}{4}\pi\right) \tag{71}$$

$$\begin{aligned}\int_{x_1}^{x} k(x')\mathrm{d}x' &= \int_{x_1}^{x} \frac{1}{\hbar}\sqrt{2m[E-V(x')]}\mathrm{d}x' \\ &= \int_0^{\xi} \frac{1}{\hbar}\sqrt{2m[E-V(x')]}\mathrm{d}\xi \left(-\frac{2m}{\hbar^2}\frac{\mathrm{d}V(x)}{\mathrm{d}x}\bigg|_{x_1}\right)^{-\frac{1}{3}} \\ &= \int_0^{\xi} \xi'^{\frac{1}{2}}\mathrm{d}\xi' = \frac{2}{3}\xi^{\frac{3}{2}}\end{aligned} \tag{72}$$

故

$$\tilde{\eta}_1 = -\frac{1}{4}\pi \tag{73}$$

$$\psi(x) = B\frac{1}{[\kappa(x)]^{\frac{1}{2}}}\cos\left[\int_{x_1}^{x}\kappa(x')\mathrm{d}x' - \frac{1}{4}\pi\right] \tag{74}$$

从 x_2 的方向看，当 $x > x_2$ 时，

$$\psi(x) = C\frac{1}{[\kappa(x)]^{\frac{1}{2}}}\exp\left[-\int_{x_2}^{x}\kappa(x')\mathrm{d}x'\right] \tag{75}$$

当 $x < x_2$ 时，

$$\psi(x) = D\frac{1}{[\kappa(x)]^{\frac{1}{2}}}\cos\left[\int_{x}^{x_2}\kappa(x')\mathrm{d}x' - \tilde{\eta}_2\right] \tag{76}$$

令

$$\xi = \left(\frac{2m}{\hbar^2}\frac{\mathrm{d}V(x)}{\mathrm{d}x}\bigg|_{x_2}\right)^{\frac{1}{3}}(x_2 - x) \tag{77}$$

其中 ξ 和 $(x_2 - x)$ 同号。薛定谔方程可化为 Airy equation

$$\frac{\mathrm{d}^2}{\mathrm{d}\xi^2}\psi + \xi\psi = 0 \tag{78}$$

当 $\xi \to \infty$ 时，

$$\psi \sim \frac{1}{\xi^{\frac{1}{4}}}\cos\left(\frac{2}{3}\xi^{\frac{3}{2}} - \frac{1}{4}\pi\right) \tag{79}$$

$$\begin{aligned}\int_{x}^{x} k(x_2)\mathrm{d}x' &= \int_{x}^{x_2} \frac{1}{\hbar}\sqrt{2m[E-V(x')]}\mathrm{d}x' \\ &= \int_{\xi}^{0} \frac{1}{\hbar}\sqrt{2m[E-V(x')]}\mathrm{d}\xi \left(-\frac{2m}{\hbar^2}\frac{\mathrm{d}V(x)}{\mathrm{d}x}\bigg|_{x_1}\right)^{-\frac{1}{3}} \\ &= \int_0^{\xi} \xi'^{\frac{1}{2}}\mathrm{d}\xi' = \frac{2}{3}\xi^{\frac{3}{2}}\end{aligned} \tag{80}$$

故

$$\tilde{\eta}_2 = \frac{1}{4}\pi \tag{81}$$

$$\psi(x) = D\frac{1}{[\kappa(x)]^{\frac{1}{2}}}\cos\left[\int_{x}^{x_2}\kappa(x')\mathrm{d}x' - \frac{1}{4}\pi\right] \tag{82}$$

我们来总结一下，当 $x > x_1$ 时

$$\psi(x) = B\frac{1}{[\kappa(x)]^{\frac{1}{2}}}\cos\left[\int_{x_1}^{x}\kappa(x')\mathrm{d}x' - \frac{1}{4}\pi\right] \tag{83}$$

当 $x < x_2$ 时

$$\psi(x) = D\frac{1}{[\kappa(x)]^{\frac{1}{2}}}\cos\left[\int_{x}^{x_2}\kappa(x')\mathrm{d}x' - \frac{1}{4}\pi\right] \tag{84}$$

这两个解本质上是同一个解

$$\int_{x_1}^{x_2}\kappa(x')\mathrm{d}x'+\int_{x_2}^{x}\kappa(x')\mathrm{d}x'-\frac{1}{4}\pi=n\pi-\left[\int_{x}^{x_2}\kappa(x')\mathrm{d}x'-\frac{1}{4}\pi\right] \tag{85}$$

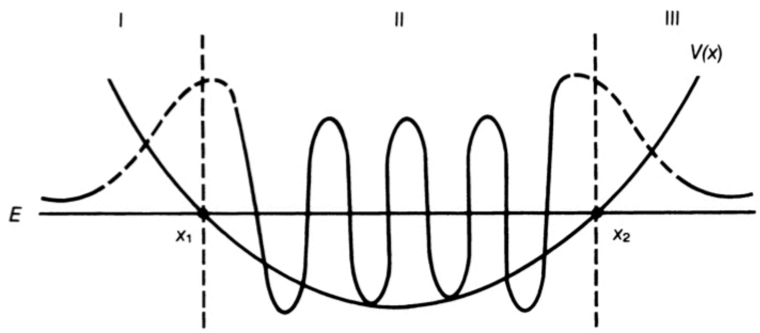
$$\int_{x_1}^{x_2}k(x)\mathrm{d}x=n\pi+\frac{1}{2}\pi=\left(n+\frac{1}{2}\right)\pi \tag{86}$$

这也是所谓的玻尔量子化条件。这个式子也可以写成另一种形式

$$p(x)=\hbar k(x) \tag{87}$$

$$\int_{x_1}^{x_2}p(x)\mathrm{d}x=\left(n+\frac{1}{2}\right)\pi\hbar \tag{88}$$

$$\oint p(x)\mathrm{d}x=(2n+1)\pi\hbar \tag{89}$$

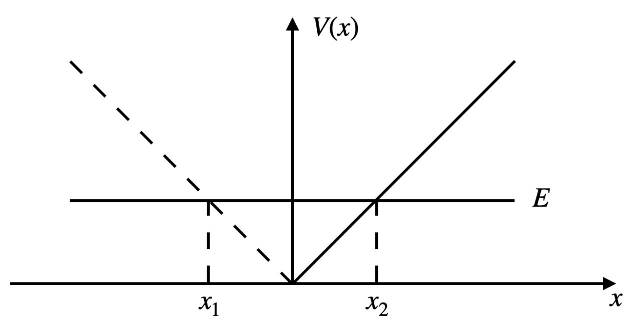


Example: The Energy Spectrum of A Ball Bouncing Up And Down Over A Hard Surface

$$V(x)=\begin{cases}mgx & x>0\\ \infty & x<0\end{cases} \tag{90}$$

将势阱进行偶延拓 $V(x)=V(-x)$

$$V(x)=mg|x| \tag{91}$$



拐点

$$x_1=-\frac{E}{mg}\qquad x_2=\frac{E}{mg} \tag{92}$$

根据初始条件，n 只取奇数。量子化条件

$$\int_{-E/mg}^{E/mg} \mathrm{d}x\sqrt{2m(E-mg|x|)} = \left(n_{\text{odd}}+\frac{1}{2}\right)\pi\hbar \qquad (n_{\text{odd}}=1,3,5,\cdots) \tag{93}$$

$$\int_{0}^{E/mg} \mathrm{d}x\sqrt{2m(E-mgx)} = \left(n-\frac{1}{4}\right)\pi\hbar \qquad (n=1,2,3,\cdots) \tag{94}$$

又

$$\begin{aligned}\int_{0}^{E/mg} \mathrm{d}x\sqrt{2m(E-mgx)} &= \frac{\sqrt{2m}}{\hbar}\int_{0}^{E/mg} \mathrm{d}x\sqrt{E-mgx} \\ &= \frac{\sqrt{2m}}{\hbar}\frac{1}{mg}\frac{2}{3}(E-mgx)^{\frac{3}{2}}\Big|_{E/mg}^{0} \\ &= \frac{\sqrt{2m}}{mg\hbar}\frac{2}{3}E^{\frac{3}{2}}\end{aligned} \tag{95}$$

$$E_n = \frac{1}{2}\left[3\left(n-\frac{1}{4}\right)\pi\right]^{\frac{2}{3}}(mg^2\hbar^2)^{\frac{1}{3}} \tag{96}$$

这个问题不需要任何近似就能分析解决，能量值可以用 Airy function 的零点来表示

$$\mathrm{Ai}(-\lambda_n) = 0 \tag{97}$$

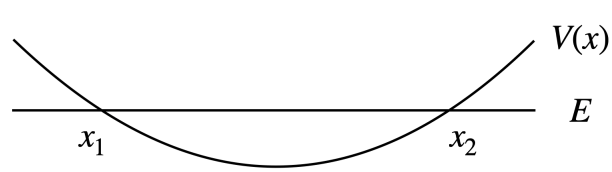
$$E_n = \left(\frac{\lambda_n}{2^{\frac{1}{3}}}\right)(mg^2\hbar^2)^{\frac{1}{3}} \tag{98}$$

对弹跳球的量子理论处理，看似与现实世界关系不大。但事实证明，这种类型的势能实际上对研究 quark-antiquark bound system (quarkonium) 的能谱具有实际意义。

n	WKB	Exact
1	2.320	2.338
2	4.082	4.088
3	5.517	5.521
4	6.784	6.787
5	7.942	7.944
6	9.021	9.023
7	10.039	10.040
8	11.008	11.009
9	11.935	11.936
10	12.828	12.829

6 Alternate Point of View

从 $x<x_2$ 到 $x>x_2$，本质上是同一个解，在实空间无法绕过 $x=x_2$ 这点，而在复空间可以绕过。所以我们接下来要做解析延拓，将解延拓成复变量的形式。



当 $x > x_2$ 时，

$$\psi(x) = \frac{C}{[\kappa(x)]^{\frac{1}{2}}} \exp\left[-\int_{x_2}^{x} \kappa(x')\mathrm{d}x'\right] \tag{99}$$

当 $x < x_2$ 时，

$$\begin{aligned}\psi(x) =& \frac{D}{[\kappa(x)]^{\frac{1}{2}}} \cos\left[\int_{x}^{x_2} \kappa(x')\mathrm{d}x' - \frac{\pi}{4}\right] \\ \sim& \frac{1}{[\kappa(x)]^{\frac{1}{2}}} \left\{\exp\left[-i\int_{x_2}^{x} \kappa(x')\mathrm{d}x' - i\frac{\pi}{4}\right] + \exp\left[i\int_{x_2}^{x} \kappa(x')\mathrm{d}x' + i\frac{\pi}{4}\right]\right\}\end{aligned} \tag{100}$$

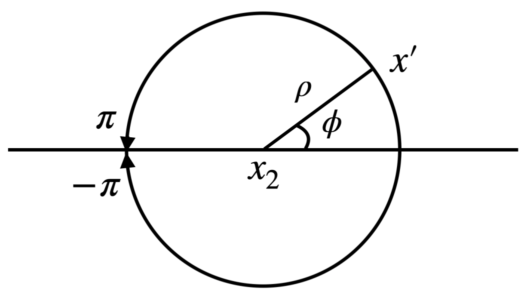
当 $x > x_2$ 时，在 $x = x_2$ 处作线性展开

$$\kappa(x') \sim \sqrt{x' - x_2} \tag{101}$$

$$\psi(x) \sim \frac{1}{(x - x_2)^{\frac{1}{4}}} \exp\left[-\int_{x_2}^{x} \sqrt{x' - x_2}\mathrm{d}x'\right] \tag{102}$$

当 $x < x_2$ 时，

$$\psi(x) \sim \frac{1}{(x_2 - x)^{\frac{1}{4}}} \left\{\exp\left[-i\int_{x_2}^{x} \sqrt{x_2 - x}\mathrm{d}x' - i\eta_2\right] + \exp\left[i\int_{x_2}^{x} \sqrt{x_2 - x}\mathrm{d}x' + i\eta_2\right]\right\} \tag{103}$$



令

$$x' - x_2 = \rho e^{i\phi} \tag{104}$$

$$k(x') \sim \sqrt{x_2 - x'} \tag{105}$$

则

$$\begin{aligned}-\int_{x_2}^{x} \mathrm{d}x'\kappa(x) = -\int_{x_2}^{x} \mathrm{d}x'\sqrt{x' - x_2} &= -\int_{x_2}^{x} \mathrm{d}x'\sqrt{(x_2 - x')e^{i\pi}} = -i\int_{x_2}^{x} \mathrm{d}x' k(x') \qquad (\text{沿 } \pi \text{ 方向延拓}) \\ &= -\int_{x_2}^{x} \mathrm{d}x'\sqrt{(x_2 - x')e^{-i\pi}} = i\int_{x_2}^{x} \mathrm{d}x' k(x') \qquad (\text{沿 } -\pi \text{ 方向延拓})\end{aligned} \tag{106}$$

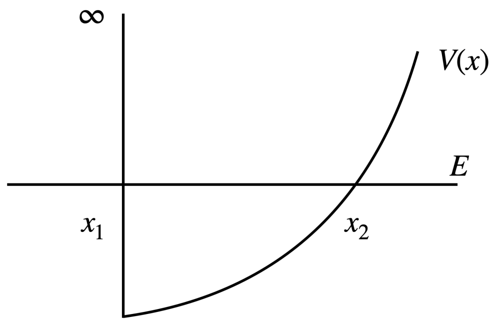
$$\begin{aligned}[\kappa(x)]^{-\frac{1}{2}} = (x - x_2)^{-\frac{1}{4}} &= \left[(x_2 - x)e^{i\pi}\right]^{-\frac{1}{4}} = [k(x)]^{-\frac{1}{2}} e^{-i\frac{\pi}{4}} \qquad (\text{沿 } \pi \text{ 方向延拓}) \\ &= \left[(x_2 - x)e^{-i\pi}\right]^{-\frac{1}{4}} = [k(x)]^{-\frac{1}{2}} e^{i\frac{\pi}{4}} \qquad (\text{沿 } -\pi \text{ 方向延拓})\end{aligned} \tag{107}$$

故

$$\eta_2 = \frac{\pi}{4} \tag{108}$$

7 Other Special Cases

Example 1



$$\psi(x_1) = 0 \tag{109}$$

当 $x > x_1$ 时

$$\psi(x) \sim \sin\left[\int_{x_1}^{x} k(x')\mathrm{d}x' + \eta\right] \tag{110}$$

当 $x \to x_1$ 时，$\psi(x) \to 0$，故 $\eta = 0$。

$$\psi(x) \sim \cos\left[\frac{\pi}{2} - \int_{x_1}^{x} k(x')\mathrm{d}x'\right] = \cos\left[\frac{\pi}{2} + \int_{x}^{x_2} k(x')\mathrm{d}x' + \int_{x_2}^{x_1} k(x')\mathrm{d}x'\right] \tag{111}$$

当 $x < x_2$ 时

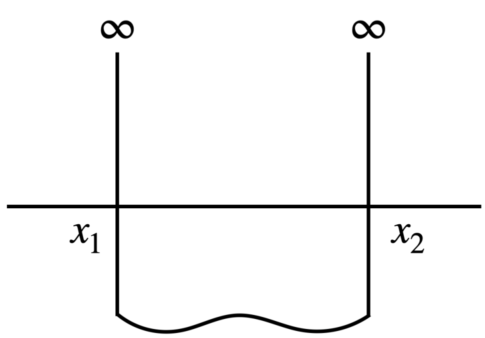
$$\psi(x) \sim \cos\left[\int_{x_2}^{x} k(x')\mathrm{d}x' - \frac{\pi}{4}\right] \tag{112}$$

这两个解本质上是同一个解

$$\int_{x_1}^{x_2} k(x')\mathrm{d}x' = \left(n - \frac{1}{4}\right)\pi \tag{113}$$

这和解析延拓的结果完全一致。

Example 2



若用玻尔量子化条件

$$\int_{x_1}^{x_2} k(x')\mathrm{d}x' = \left(n + \frac{1}{2}\right)\pi \tag{114}$$

将得到错误的结果，因为在 x_1 和 x_2 处都不满足 WKB 近似条件，即 $V(x)$ 变化缓慢。这时我们需要重新讨论，做特殊处理。

当 $x > x_1$ 时

$$\psi(x) \sim \sin\left[\int_{x_1}^{x} k(x')\mathrm{d}x'\right] \tag{115}$$

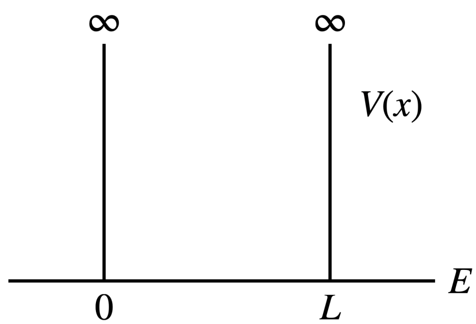
当 $x < x_2$ 时

$$\psi(x) \sim \sin\left[\int_{x}^{x_2} k(x')\mathrm{d}x'\right] = \sin\left[\int_{x}^{x_1} k(x')\mathrm{d}x' + \int_{x_1}^{x_2} k(x')\mathrm{d}x'\right] \tag{116}$$

$$\int_{x_1}^{x_2} k(x')\mathrm{d}x' = n\pi \tag{117}$$

$$\oint p(x)\mathrm{d}x = 2n\pi\hbar = nh \tag{118}$$

这也就是索末菲量子化条件。

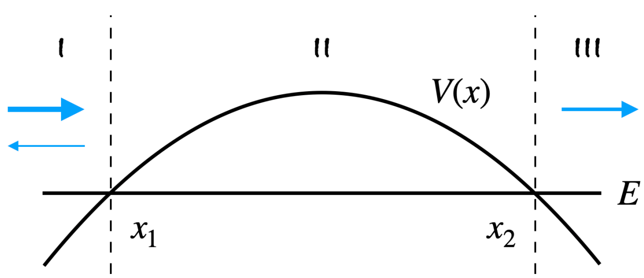


利用索末菲量子化条件

$$2\int_0^L \sqrt{2mE}\mathrm{d}x = nh \tag{119}$$

$$E = \frac{n^2h^2}{8mL^2} \tag{120}$$

8 tunneling 势垒贯穿



- 在 I 区域

$$\psi(x) = \frac{1}{\sqrt{k(x)}}\cos\left[\int_{x_1}^{x} k(x')\mathrm{d}x' - \frac{\pi}{4}\right] \tag{121}$$

- 在 II 区域

$$\psi(x) = \frac{1}{\sqrt{\kappa(x)}}\exp\left[-\int_{x_1}^{x} \kappa(x')\mathrm{d}x'\right] + c_0\frac{1}{\sqrt{\kappa(x)}}\exp\left[\int_{x_1}^{x} \kappa(x')\mathrm{d}x'\right] \tag{122}$$

由于 $|c_0| \ll 1$

$$\psi(x) \doteq \frac{1}{\sqrt{\kappa(x)}}\exp\left[-\int_{x_1}^{x} \kappa(x')\mathrm{d}x'\right] \tag{123}$$

- 在 III 区域

$$\psi(x)=\frac{c}{\sqrt{k(x)}}\exp\left[i\int_{x_1}^{x}k(x')\mathrm{d}x'+i\frac{\pi}{4}\right] \tag{124}$$

透射波几率流密度

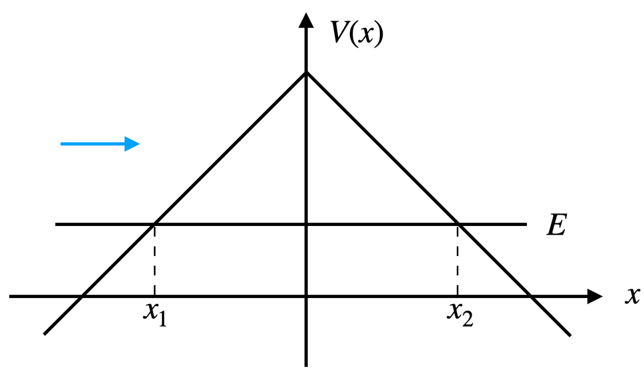
$$J=k(x_2)|\psi(x_2)|^2\sim\exp\left[-2\int_{x_1}^{x_2}\kappa(x')\mathrm{d}x'\right] \tag{125}$$

隧穿因子 (tunneling factor)

$$T\propto\exp\left[-2\int_{x_1}^{x_2}\kappa(x)\mathrm{d}x\right]=\exp\left\{-2\int_{x_1}^{x_2}\frac{1}{\hbar}\sqrt{2m[V(x)-E]}\mathrm{d}x\right\} \tag{126}$$

Example

$$V(x)=\begin{cases}V_0-mgx & x>0\\ V_0+mgx & x<0\end{cases} \tag{127}$$

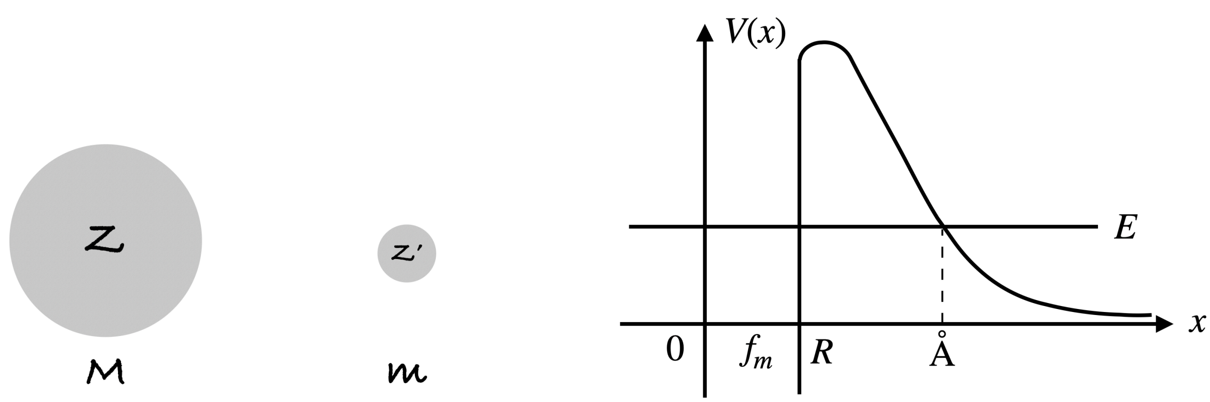


$$T=\exp\left[-2\int_{x_1}^{x_2}\kappa(x)\mathrm{d}x\right]=\exp\left[-4\int_{0}^{x_2}\frac{\sqrt{2m}}{\hbar}\sqrt{V_0-mgx-E}\mathrm{d}x\right]=\exp\left[-\frac{8}{3}\sqrt{\frac{2m}{\hbar}}\frac{1}{mg}(V_0-E)^{\frac{3}{2}}\right] \tag{128}$$

Example: The α Decay of Nuclei

$$V(r)=\frac{ZZ'e^2}{r} \tag{129}$$

$$r_1\sim f_m\qquad r_2\sim\mathring{A}\qquad r_2\gg r_1 \tag{130}$$



这个问题具有球对称性，因此我们只考虑它的径向

$$\psi_{n,l,m}(r,\theta,\phi)=\frac{\chi(r)}{r}Y_{l,m}(\theta,\phi) \tag{131}$$

$$-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}r^2}\chi(r)+\left[\frac{ZZ'e^2}{r}+\frac{l(l+1)}{2\mu r^2}\right]\chi(r)=E\chi(r) \tag{132}$$

有效势

$$V_{\text{eff}}(r)=\frac{ZZ'e^2}{r}+\frac{l(l+1)}{2\mu r^2} \tag{133}$$

$$V(r)=\frac{ZZ'e^2}{r} \tag{134}$$

$$\begin{aligned} T&=\exp\left\{-2\int_{r_1}^{r_2}\frac{1}{\hbar}\sqrt{2\mu[V_{\text{eff}}(r)-E]}\mathrm{d}r\right\} \\ &=\exp\left\{-2\int_{r_1}^{r_2}\frac{1}{\hbar}\sqrt{2\mu\left[\frac{ZZ'e^2}{r}+\frac{l(l+1)}{2\mu r^2}-E\right]}\mathrm{d}r\right\}\end{aligned} \tag{135}$$

$$r_2=\frac{ZZ'e^2}{E} \tag{136}$$

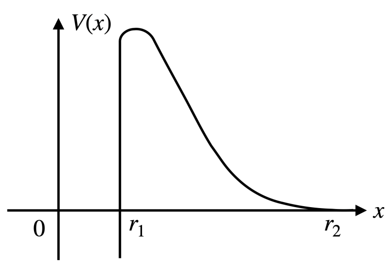
1. $E\neq 0,\ l=0$

$$\begin{aligned}&\frac{1}{\hbar}\int_{r_1}^{r_2}\sqrt{2\mu[V_{\text{eff}}(r)-E]}\mathrm{d}r=\frac{\sqrt{2\mu}}{\hbar}\int_{r_1}^{r_2}\sqrt{\frac{ZZ'e^2}{r}-E}\mathrm{d}r \\ =&\frac{\pi ZZ'e^2}{\hbar\sqrt{\frac{2E}{\mu}}}\left(1-\frac{2}{\pi}\sin^{-1}\sqrt{\frac{ER}{ZZ'e^2}}\right)-\frac{\sqrt{2\mu E}R}{\hbar}\left(\frac{ZZ'e^2}{ER}-1\right)^{\frac{1}{2}}\end{aligned} \tag{137}$$

2. $E=0,\ l=0$

$$T=\exp\left\{-\int_{r_1}^{r_2}\frac{2}{\hbar}\sqrt{2\mu V(r)}\mathrm{d}r\right\} \tag{138}$$

   (a) If $V(x)$ has a finite range

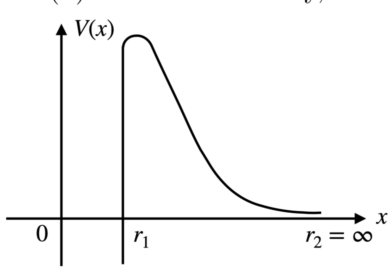


$$\int_{r_1}^{r_2}\frac{2}{\hbar}\sqrt{2\mu V(r)}\mathrm{d}r=\text{finite} \tag{139}$$

$$T\neq 0 \tag{140}$$

能发生隧穿。

   (b) If $V(x)$ extends to infinity, but falls off faster than $\frac{1}{r^2}$



$$\int_{r_1}^{r_2}\frac{2}{\hbar}\sqrt{2\mu V(r)}\mathrm{d}r<\int_{r_1}^{\infty}\frac{2}{\hbar}\sqrt{2\mu}\frac{1}{r^{2+\varepsilon}}\mathrm{d}r=\text{finite} \tag{141}$$

$$T\neq 0 \tag{142}$$

能发生隧穿。

   (c) If $V(x)$ extends to infinity, but falls off like $\frac{1}{r^2}$

$$\int_{r_1}^{r_2}\frac{2}{\hbar}\sqrt{2\mu V(r)}\mathrm{d}r\sim\int^{\infty}\frac{1}{r}\mathrm{d}r\to\infty \tag{143}$$

$$T = 0 \tag{144}$$

不能发生隧穿。

3. $E = 0,\ l > 0$

$$T = \exp\left\{-2\int_{r_1}^{r_2}\frac{1}{\hbar}\sqrt{2\mu\left[\frac{ZZ'e^2}{r}+\frac{l(l+1)}{2\mu r^2}\right]}\mathrm{d}r\right\} \tag{145}$$

$$\int_{r_1}^{r_2}\frac{2}{\hbar}\sqrt{2\mu\left[\frac{ZZ'e^2}{r}+\frac{l(l+1)}{2\mu r^2}\right]}\mathrm{d}r \geq \int_{r_1}^{r_2}\frac{2}{\hbar}\frac{\sqrt{l(l+1)}}{r}\mathrm{d}r \overset{r_2\to\infty}{=} \text{infinity} \tag{146}$$

$$T = 0 \tag{147}$$

不能发生隧穿。