《量子力学教程》课后习题——第二章 波函数和薛定谔方程

物理（4+4）1801 胡喜平 学号 U201811966

网站 https://hxp.plus/ 邮件 hxp201406@gmail.com

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2.1 证明在定态中，概率流密度与时间无关。

解 定态波函数为

$$\psi\left(r,t\right)=\psi\left(r\right)\exp\left[-\frac{iE}{\hbar}t\right]$$

概率流密度为

$$\begin{aligned}J&=\frac{\hbar}{2i\mu}\left|\psi\left(r\right)\right|^2\nabla\ln\left\{\frac{\psi\left(r\right)}{\psi^*\left(r\right)}\exp\left[-\frac{2iE}{\hbar}t\right]\right\}=\frac{\hbar}{2i\mu}\left|\psi\left(r\right)\right|^2\nabla\left\{\ln\left[\frac{\psi\left(r\right)}{\psi^*\left(r\right)}\right]+\frac{2iEt}{\hbar}\right\}\\&=\frac{\hbar}{2i\mu}\left|\psi\left(r\right)\right|^2\nabla\ln\left[\frac{\psi\left(r\right)}{\psi^*\left(r\right)}\right]\end{aligned}$$

与时间无关。

2.2 由下列两定态波函数计算概率流密度。

$$\psi_1=\frac{1}{r}\exp\left[ikr\right]\qquad\qquad\psi_2=\frac{1}{r}\exp\left[-ikr\right]$$

从所得结果说明 ψ_1 表示向外传播的球面波，ψ_2 表示向内（即向原点）传播的球面波。

解

$$\vec{J}_1=\frac{\hbar}{2i\mu}\left|\psi\right|^2\nabla\ln\frac{\psi}{\psi^*}=\frac{\hbar}{2i\mu}\frac{1}{r^2}\nabla\left(2ikr\right)=\frac{\hbar k}{\mu r^2}\vec{e}_r$$

$$\vec{J}_2=\frac{\hbar}{2i\mu}\left|\psi\right|^2\nabla\ln\frac{\psi}{\psi^*}=\frac{\hbar}{2i\mu}\frac{1}{r^2}\nabla\left(-2ikr\right)=-\frac{\hbar k}{\mu r^2}\vec{e}_r$$

ψ_1 是沿着 $\vec{e}_r$ 方向传播的，ψ_2 是沿着 $\vec{e}_r$ 相反方向传播的。

2.3 一粒子在一维势场

$$U(x)=\begin{cases}\infty & x<0\\ 0 & 0\le x\le a\\ \infty & x>a\end{cases}$$

中运动，求粒子的能级和对应的波函数。

解 在 $0<x<a$ 时，薛定谔方程

$$-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}=E\psi$$

即

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}-\frac{\hbar^2}{2\mu E}\psi=0$$

设

$$\psi=A\cos\alpha x+B\sin\alpha x$$

代入解得

$$\psi=A\cos\alpha x+B\sin\alpha x\qquad\qquad \alpha=\sqrt{\frac{2\mu E}{\hbar^2}}$$

由波函数连续条件

$$\psi|_{x=0}=\psi|_{x=a}=0$$

得到

$$A=0\qquad\qquad B\sin\alpha a=0\Rightarrow\sqrt{\frac{2\mu E}{\hbar^2}}=\alpha=\frac{n\pi}{a}\Rightarrow E_n=\frac{\pi^2\hbar^2}{2\mu a^2}n^2$$

由波函数归一化条件

$$\int_0^a\left[B\sin\frac{n\pi}{a}x\right]^2\mathrm{d}x=B^2\int_0^a\frac{1-\cos\dfrac{2n\pi}{a}x}{2}\mathrm{d}x=\frac{B^2}{2}a=1$$

解得

$$B = \sqrt{\frac{2}{a}}$$

因此波函数为

$$\psi_n\left(x\right) = \begin{cases} \sqrt{\frac{2}{a}} \sin \frac{n\pi}{a} x & 0 < x < a \\ 0 & x < 0, x > a \end{cases}$$

2.4 证明下式中的归一化因子是 $A' = \frac{1}{\sqrt{a}}$

$$\psi_n = \begin{cases} A' \sin \frac{n\pi}{2a} \left(x + a\right) & |x| < a \\ 0 & |x| \geq a \end{cases}$$

解

$$\int_{-a}^{a} \left[A' \sin \frac{n\pi}{a} \left(x + a\right)\right]^2 \mathrm{d}x = \frac{A'^2}{2} \int_{-a}^{a} \left[1 - \cos \frac{2n\pi}{a} \left(x + a\right)\right] \mathrm{d}x = A'^2 a = 1 \Rightarrow A' = \frac{1}{\sqrt{a}}$$

2.5 求一维谐振子处在第一激发态时概率最大的位置。

解 对应能量 E_n 的波函数是

$$\psi_n\left(\xi\right) = N_n \exp\left[-\frac{\xi^2}{2}\right] H_n\left(\xi\right) \qquad \xi = \alpha x \qquad N_n = \left(\frac{\alpha}{\pi^{\frac{1}{2}} 2^n n!}\right)^{\frac{1}{2}}$$

$n = 1$ 时

$$\psi_1\left(x\right) = \left(\frac{\alpha}{2\sqrt{\pi}}\right)^{\frac{1}{2}} \exp\left[-\frac{\alpha^2}{2} x^2\right] \cdot 2\alpha x$$

概率为

$$w\left(x\right) = \left|\psi\left(x\right)\right|^2 = \frac{2\alpha^3}{\sqrt{\pi}} x^2 \exp\left[-\alpha^2 x^2\right]$$

对概率求导数

$$\frac{\mathrm{d}w\left(x\right)}{\mathrm{d}x} = \frac{4\alpha^3}{\sqrt{\pi}} \left[x\left(1 - \alpha^2 x^2\right)\right] \exp\left[-a^2 x^2\right]$$

$$\frac{\mathrm{d}^2 w\left(x\right)}{\mathrm{d}x^2} = \frac{4\alpha^3}{\sqrt{\pi}} \left(2\alpha^4 - 5\alpha^2 x^2 + 1\right) \exp\left[-\alpha^2 x^2\right]$$

只有当 $x = \pm\frac{1}{\alpha}$ 时，$\frac{\mathrm{d}w\left(x\right)}{\mathrm{d}x} = 0$ 且 $\frac{\mathrm{d}^2 w\left(x\right)}{\mathrm{d}x^2} < 0$，因此最大概率位置 $x = \pm\frac{1}{\alpha}$

2.6　在一维势场中运动的粒子，势能对原点对称：$U(-x)=U(x)$，证明粒子的定态波函数具有确定的宇称。

解　薛定谔方程为

$$\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2}+\frac{2\mu}{\hbar^2}\left[E-U(x)\right]\psi(x)=0$$

$$\frac{\mathrm{d}^2\psi(-x)}{\mathrm{d}x^2}+\frac{2\mu}{\hbar^2}\left[E-U(x)\right]\psi(-x)=0$$

$\psi(x)$ 和 $\psi(-x)$ 是一个方程的解，它们的线性组合也是方程的解。因此下面两个方程是薛定谔方程的解

$$\psi_e(x)=\psi(x)+\psi(-x)$$

$$\psi_o(x)=\psi(x)-\psi(-x)$$

其中 $\psi_e(x)$ 是偶函数，$\psi_o(x)$ 是奇函数。因此有确定的宇称。

2.7　一粒子在一维深势阱

$$U(x)=\begin{cases}V_0>0 & |x|>a\\ 0 & |x|\le a\end{cases}$$

中运动，求束缚态（$0<E<V_0$）的能级所满足的方程。

解　（这个方法参考了附在后面的文档，文档节选自 David A.B. Miller 的 Quantum Mechanics，我觉得这个方法比较有意思就研究了下）

设波函数的解为

$$\psi(x)=\begin{cases}G\exp(\kappa x) & x<-a\\ A\sin kx+B\cos kx & -a<x<a\\ F\exp(-\kappa x)\end{cases}$$

其中

$$\kappa=\sqrt{2m\left(V_0-E\right)/\hbar^2}$$
$$k=\sqrt{2mE/\hbar^2}$$

设

$$
\begin{aligned}
X_L &= \exp\left(-\kappa a\right) \\
S_L &= \sin\left(ka\right) \\
C_L &= \cos\left(ka\right)
\end{aligned}
$$

连续性给出

$$
\begin{aligned}
GX_L &= -AS_L + BC_L \\
FX_L &= AS_L + BC_L \\
\frac{\kappa}{k}GX_L &= AC_L + BS_L \\
-\frac{\kappa}{k}FX_L &= AC_L - BS_L
\end{aligned}
$$

解出

$$
\begin{aligned}
2BC_L &= \left(F+G\right)X_L \\
2BS_L &= \frac{\kappa}{k}\left(F+G\right)X_L
\end{aligned}
$$

有两组解

$$
\begin{aligned}
\tan ka &= \frac{\kappa}{k} \quad F \neq -G \\
-\cot ka &= \frac{\kappa}{k} \quad F \neq G
\end{aligned}
$$

其中 $F=G$ 和 $F=-G$ 必须满足一个，否则无解。定义

$$
\begin{aligned}
E_1^\infty &= \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2 \\
\varepsilon &= \frac{E}{E_1^\infty} \\
v_0 &= \frac{V_0}{E_1^\infty}
\end{aligned}
$$

则

$$
\begin{aligned}
\frac{\kappa}{k} &= \sqrt{\frac{v_0-\varepsilon}{\varepsilon}} \\
ka &= \frac{\pi}{2}\sqrt{\frac{E}{E_1^\infty}} = \frac{\pi}{2}\sqrt{\varepsilon} \\
\kappa a &= \frac{\pi}{2}\sqrt{\frac{V_0-E}{E_1^\infty}} = \frac{\pi}{2}\sqrt{v_0-\varepsilon}
\end{aligned}
$$

定义

$$
\begin{aligned}
c_L &= \frac{C_L}{X_L} = \frac{\cos\left(\pi\sqrt{\varepsilon}/2\right)}{\exp\left(-\pi\sqrt{v_0-\varepsilon}/2\right)} \\
s_L &= \frac{S_L}{X_L} = \frac{\sin\left(\pi\sqrt{\varepsilon}/2\right)}{\exp\left(-\pi\sqrt{v_0-\varepsilon}/2\right)}
\end{aligned}
$$

当 $F=G$ 时

$$
\sqrt{\varepsilon}\tan\left(\frac{\pi}{2}\sqrt{\varepsilon}\right) = \sqrt{v_0-\varepsilon}
$$

波函数为

$$
\psi\left(x\right) = \begin{cases}
Bc_L\exp\left(2\pi\sqrt{v_0-\varepsilon}\cdot\dfrac{x}{a}\right) \\
B\cos\left(2\pi\sqrt{\varepsilon}\cdot\dfrac{x}{a}\right) \\
Bc_L\exp\left(-2\pi\sqrt{v_0-\varepsilon}\cdot\dfrac{x}{a}\right)
\end{cases}
$$

当 $F=-G$ 时

$$
-\sqrt{\varepsilon}\cot\left(\frac{\pi}{2}\sqrt{\varepsilon}\right) = \sqrt{v_0-\varepsilon}
$$

波函数为

$$
\psi\left(x\right) = \begin{cases}
-As_L\exp\left(2\pi\sqrt{v_0-\varepsilon}\cdot\dfrac{x}{a}\right) \\
A\sin\left(2\pi\sqrt{\varepsilon}\cdot\dfrac{x}{a}\right) \\
As_L\exp\left(-2\pi\sqrt{v_0-\varepsilon}\cdot\dfrac{x}{a}\right)
\end{cases}
$$

2.8 分子间的范德瓦尔斯力所产生的势能可以近似地表示为

$$
U\left(x\right) = \begin{cases}
\infty & x<0 \\
U_0 & 0\le x<a \\
-U_1 & a\le x\le b \\
0 & b<x
\end{cases}
$$

求束缚态的能级所满足的方程。

解 设波函数的解为

$$\psi\left(x\right)=\begin{cases}0 & x<0\\ A\exp\left(\kappa_0 x\right)-A\exp\left(-\kappa_0 x\right) & 0<x<a\\ C\sin kx+D\cos kx & a<x<b\\ G\exp\left(-\kappa_2 x\right) & x>b\end{cases}$$

其中

$$\begin{aligned}\kappa_0&=\sqrt{2m\left(U_0-E\right)/\hbar^2}\\ k&=\sqrt{2m\left(U_1+E\right)/\hbar^2}\\ \kappa_2&=\sqrt{-2mE/\hbar^2}\end{aligned}$$

波函数边界连续条件给出

$$\begin{aligned}&A\exp\left(\kappa_0 a\right)-A\exp\left(-\kappa_0 a\right)=C\sin ka+D\cos ka\\ &\kappa_0 A\exp\left(\kappa_0 a\right)+\kappa_0 A=kC\cos ka-kD\sin ka\\ &G\exp\left(-\kappa_2 b\right)=C\sin kb-D\cos kb\\ &-\kappa_2 G\exp\left(-\kappa_2 b\right)=kC\cos kb-kD\sin kb\end{aligned}$$

即

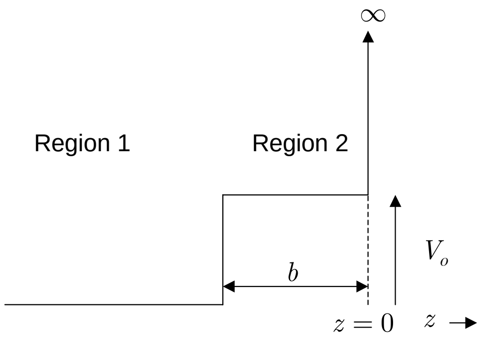
$$\begin{bmatrix}2\sinh\kappa_0 a & -\sin ka & -\cos ka & 0\\ 2\kappa_0\cosh\kappa_0 a & -k\cos ka & k\sin ka & 0\\ 0 & -\sin kb & -\cos kb & \exp\left(-\kappa_2 b\right)\\ 0 & -k\cos kb & k\sin kb & -\kappa_2\exp\left(-\kappa_2 b\right)\end{bmatrix}\begin{bmatrix}A\\ C\\ D\\ G\end{bmatrix}=0$$

波函数有解的条件是

$$\begin{vmatrix}2\sinh\kappa_0 a & -\sin ka & -\cos ka & 0\\ 2\kappa_0\cosh\kappa_0 a & -k\cos ka & k\sin ka & 0\\ 0 & -\sin kb & -\cos kb & \exp\left(-\kappa_2 b\right)\\ 0 & -k\cos kb & k\sin kb & -\kappa_2\exp\left(-\kappa_2 b\right)\end{vmatrix}$$

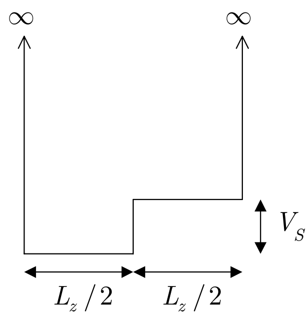
即能量需满足关系

$$\tan k\left(b-a\right)=\frac{k\kappa_0\coth\kappa_0 a+k\kappa_2}{k^2-\kappa_0\kappa_2\coth\kappa_0 a}$$



(i) Show that the wavefunction in Region 2 may be written in the form $\psi(z) = C\sin(fz)$ where C is a complex constant and f is a real constant.
(ii) What is the magnitude of the wave amplitude of the reflected wave (i.e., the wave propagating to the left)?
(iii) Find an expression for C in terms of E, V_o, and b.
(iv) Taking $V_o =$ 1 eV, and $b =$ 10 Å, sketch $|C|^2$ as a function of energy from 1.1 eV to 3 eV.
(v) Sketch the (relative) probability density in the structure at $E =$ 1.356 eV.
(vi) Provide an explanation for the form of the curve in part (iv).

2.8.7 Consider an electron in the infinitely deep one-dimensional "stepped" potential well shown in the figure. The potential step is of height V_S and is located in the middle of the well, which has total width L_z. V_S is substantially less than $(\hbar^2 / 2m_o)(\pi / L_z)^2$.



(i) Presuming that this problem can be solved, and that it results in a solution for some specific eigenenergy E_S, state the functional form of the eigenfunction solutions in each half of the well, being explicit about the values of any propagation constants or decay constants in terms of the eigenenergy E_S, the step height V_S, and the well width L_z. [Note: do not attempt a full solution of this problem – it does not have simple closed-form solutions for the eigenenergies. Merely state what the form of the solutions in each half would be if we had found an eigenenergy E_S.]
(ii) Sketch the form of the eigenfunctions (presuming we have chosen to make them real functions) for each of the first two states of this well. In your sketch, be explicit about whether any zeros in these functions are in the left half, the right half, or exactly in the middle. [You may exaggerate differences between these wavefunctions and those of a simply infinitely deep well for clarity.]
(iii) State whether each of these first two eigenfunctions have definite parity with respect to the middle of the structure, and, if so, whether that parity is even or odd.
(iv) Sketch the form of the probability density for each of the two states.
(v) State, for each of these eigenfunctions, whether the electron is more likely to be found in the left or the right half of the well.

2.9 Particle in a finite potential well

Now that we have understood the interaction of a quantum mechanical wave with a finite barrier, we can consider a particle in a "square" potential well of finite depth. This is a more realistic problem than the "infinite" (i.e., infinitely deep or with infinitely high barriers) square potential well. We presume a potential structure as shown in Fig. 2.6.

Here we have chosen the origin for the z position to be in the middle of the potential well (in contrast to the infinite well above where we chose one edge of the well). Such a choice makes no difference to the final results, but is mathematically more convenient now.

Such a problem is relatively straightforward to solve. Indeed, it is one of the few non-trivial quantum mechanical problems that can be solved analytically with relatively simple algebra and elementary functions, so it is a useful example to go through completely. It also has a close correspondence with actual problems in the design of semiconductor quantum well structures.

We consider for the moment to the case where $E < V_o$. Such solutions are known as bound states. For such energies, the particle is in some sense "bound" to the well. It certainly does not have enough energy classically to be found outside the well.

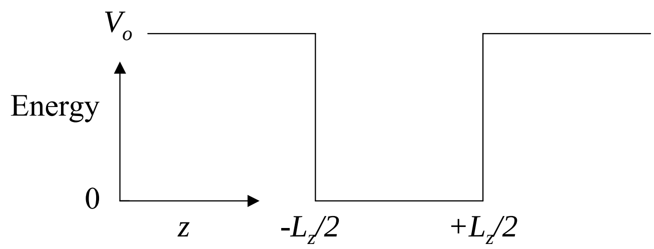


Fig. 2.6. A finite square potential well.

We know the nature of the solutions in the barriers (exponential decays away from the potential well) and in the well (sinusoidal), and we know the boundary conditions that link these solutions. We first need to find the values of the energy for which there are solutions to the Schrödinger equation, then deduce the corresponding wavefunctions.

The form of Schrödinger's equation in the potential well is the same as we had for the infinite well (i.e., Eq. (2.22), and the solutions are of the same form (i.e., Eq. (2.24)), though the valid energies E and the corresponding values of k ($=\sqrt{2mE/\hbar^2}$) will be different from the infinite well case. The form of the solution in the barrier is an exponential one as discussed above, except that the solution in the left barrier will be exponentially decaying to the left so that it does not grow as we move further away from the well. Hence, formally, the solutions are of the form

$$\psi(z) = G\exp(\kappa z),\ z < -L_z/2$$

$$\psi(z) = A\sin kz + B\cos kz,\ -L_z/2 < z < L_z/2 \tag{2.48}$$

$$\psi(z) = F\exp(-\kappa z),\ z > L_z/2$$

where the amplitudes A, B, F, G, and the energy E (and consequently k, and $\kappa = (2m(V_o - E)/\hbar^2)^{1/2}$) are constants to be determined. For simplicity of notation, we choose to write

$$X_L = \exp(-\kappa L_z/2),\ S_L = \sin(kL_z/2),\ C_L = \cos(kL_z/2)$$

so the boundary conditions give, from continuity of the wavefunction

$$GX_L = -AS_L + BC_L \tag{2.49}$$

$$FX_L = AS_L + BC_L \tag{2.50}$$

and from continuity of the derivative of the wavefunction

$$\frac{\kappa}{k}GX_L = AC_L + BS_L \tag{2.51}$$

$$-\frac{\kappa}{k}FX_L = AC_L - BS_L \tag{2.52}$$

Adding Eqs. (2.49) and (2.50) gives

$$2BC_L = (F+G)X_L \tag{2.53}$$

Subtracting Eq. (2.52) from Eq. (2.51) gives

$$2BS_L = \frac{\kappa}{k}(F+G)X_L \tag{2.54}$$

As long as $F \neq -G$, we can divide Eq. (2.54) by Eq. (2.53) to obtain

$$\tan(kL_z/2) = \kappa/k \tag{2.55}$$

Alternatively, subtracting Eq. (2.49) from Eq. (2.50) gives

$$2AS_L = (F-G)X_L \tag{2.56}$$

and adding Eqs. (2.51) and (2.52) gives

$$2AC_L = -\frac{\kappa}{k}(F-G)X_L \tag{2.57}$$

Hence, as long as $F \neq G$, we can divide Eq. (2.57) by Eq. (2.56) to obtain

$$-\cot(kL_z/2) = \kappa/k \tag{2.58}$$

For any situation other than $F = G$ (which leaves Eq. (2.55) applicable but Eq. (2.58) not) or $F = -G$ (which leaves Eq. (2.58) applicable but Eq. (2.55) not), the two relations (2.55) and (2.58) would contradict each other, so the only possibilities are (i) $F = G$ with relation (2.55), and (ii) $F = -G$ with relation (2.58).

For $F = G$, we see from Eqs. (2.56) and (2.57) that $A = 0$,[31] so we are left with only the cosine wavefunction in the well, and the overall wavefunction is symmetrical from left to right (i.e., has even parity). Similarly, for $F = -G$, $B = 0$, we are left only with the sine wavefunction in the well, and the overall wavefunction is antisymmetric from left to right (i.e., has odd parity). Hence, we are left with two sets of solutions.

To write these solutions more conveniently, we change notation. We define a useful energy unit, the energy of the first level in the infinite potential well of the same width L_z,

$$E_1^\infty = \frac{\hbar^2}{2m}\left(\frac{\pi}{L_z}\right)^2 \tag{2.59}$$

and define a dimensionless energy

$$\varepsilon \equiv E/E_1^\infty \tag{2.60}$$

and a dimensionless barrier height

$$v_o \equiv V_o/E_1^\infty \tag{2.61}$$

Consequently,

$$\frac{\kappa}{k} = \sqrt{\frac{V_o - E}{E}} = \sqrt{\frac{v_o - \varepsilon}{\varepsilon}} \tag{2.62}$$

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[31] Note formally that C_L and S_L cannot both be zero at the same time, so the only way of satisfying both of these equations is for A to be zero.

$$\frac{kL_z}{2} = \frac{\pi}{2}\sqrt{\frac{E}{E_1^\infty}} = \frac{\pi}{2}\sqrt{\varepsilon} \tag{2.63}$$

$$\frac{\kappa L_z}{2} = \frac{\pi}{2}\sqrt{\frac{V_o - E}{E_1^\infty}} = \frac{\pi}{2}\sqrt{v_o - \varepsilon} \tag{2.64}$$

We can also conveniently define two quantities that will appear in the wavefunctions

$$c_L = \frac{C_L}{X_L} = \frac{\cos(kL_z/2)}{\exp(-\kappa L_z/2)} = \frac{\cos\left(\pi\sqrt{\varepsilon}/2\right)}{\exp\left(-\pi\sqrt{v_o - \varepsilon}/2\right)} \tag{2.65}$$

$$s_L = \frac{S_L}{X_L} = \frac{\sin(kL_z/2)}{\exp(-\kappa L_z/2)} = \frac{\sin\left(\pi\sqrt{\varepsilon}/2\right)}{\exp\left(-\pi\sqrt{v_o - \varepsilon}/2\right)} \tag{2.66}$$

and it will be convenient to define a dimensionless distance

$$\zeta = \mathrm{z}/L_z \tag{2.67}$$

We can therefore write the two sets of solutions as follows.

Symmetric solution

The allowed energies satisfy

$$\sqrt{\varepsilon}\tan\left(\frac{\pi}{2}\sqrt{\varepsilon}\right) = \sqrt{v_o - \varepsilon} \tag{2.68}$$

The wavefunctions are

$$\begin{aligned}
\psi(\zeta) &= Bc_L \exp\left(\pi\sqrt{v_o - \varepsilon}\zeta\right), \ \zeta < -1/2 \\
\psi(\zeta) &= B\cos\left(\pi\sqrt{\varepsilon}\zeta\right), \ -1/2 < \zeta < 1/2 \\
\psi(\zeta) &= Bc_L \exp\left(-\pi\sqrt{v_o - \varepsilon}\zeta\right), \ \zeta > 1/2
\end{aligned} \tag{2.69}$$

Antisymmetric solution

The allowed energies satisfy

$$-\sqrt{\varepsilon}\cot\left(\frac{\pi}{2}\sqrt{\varepsilon}\right) = \sqrt{v_o - \varepsilon} \tag{2.70}$$

The wavefunctions are

$$\begin{aligned}
\psi(\zeta) &= -As_L \exp\left(\pi\sqrt{v_o - \varepsilon}\zeta\right), \zeta < -1/2 \\
\psi(\zeta) &= A\sin\left(\pi\sqrt{\varepsilon}\zeta\right), \ -1/2 < \zeta < 1/2 \\
\psi(\zeta) &= As_L \exp\left(-\pi\sqrt{v_o - \varepsilon}\zeta\right), \ \zeta > 1/2
\end{aligned} \tag{2.71}$$