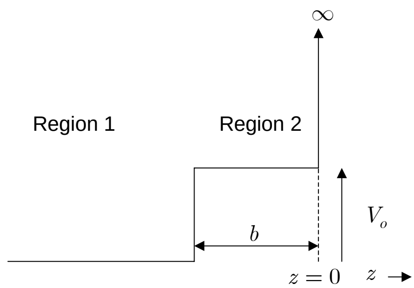
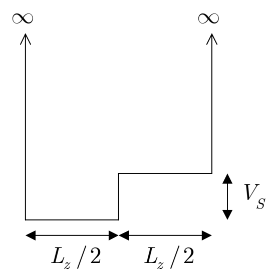


(i) Show that the wavefunction in Region 2 may be written in the form $\psi(z) = C\sin(fz)$ where C is a complex constant and f is a real constant.
(ii) What is the magnitude of the wave amplitude of the reflected wave (i.e., the wave propagating to the left)?
(iii) Find an expression for C in terms 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.

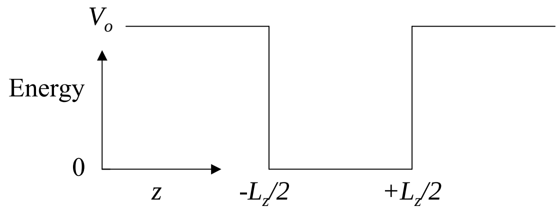


Fig. 2.6. A finite square potential well.

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

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

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

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

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

$$GX_L = -AS_L + BC_L \qquad (2.49)$$

$$FX_L = AS_L + BC_L \qquad (2.50)$$

and from continuity of the derivative of the wavefunction

$$\frac{\kappa}{k}GX_L = AC_L + BS_L \qquad (2.51)$$

$$-\frac{\kappa}{k}FX_L = AC_L - BS_L \qquad (2.52)$$

Adding Eqs. (2.49) and (2.50) gives

$$2BC_L = (F+G)X_L \qquad (2.53)$$

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

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

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

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

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

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

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

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

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

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

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,

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

[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

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