Particle in a finite-depth 1D Box (see Engel, problem P5.1)

Consider the potential energy function depicted in Fig. 1, namely a box of width a with a finite depth V_0.

This potential is piece-wise constant (has a constant value in each region I, II and III).

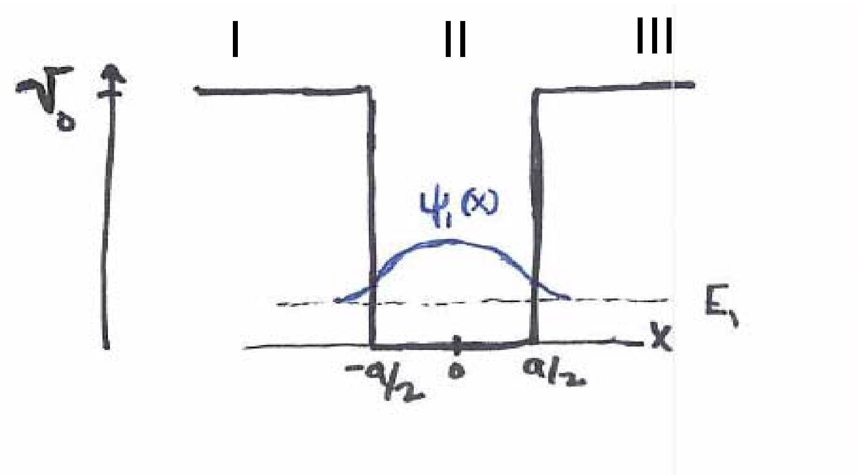


Fig. 1: Finite-depth 1D box. Ground state energy eigenfunction and energy level are sketched schematically.

Thus, we can solve the Schrödinger Equation in regions I, II, III independently, and then piece them together … see below.

Exploit the symmetry of the potential to seek solutions of even and odd parity separately.

Focus here on the even-parity solutions. An even-parity eigenfunction corresponding to energy eigenvalue E must take the form

$$\psi_I(x) = Ae^{\kappa x}$$

$$\psi_{II}(x) = \cos(kx)$$

$$\psi_{III}(x) = Ae^{-\kappa x}$$

with $k(E) \equiv \sqrt{2mE}/\hbar$ and $\kappa(E) \equiv \sqrt{2m(V_0 - E)}/\hbar$.

The allowed values of E (and the corresponding values of A) are determined by matching $\psi(x)$ and $d\psi(x)/dx$ at $x = \pm a/2$.

This leads to the following transcendental equation, which is effectively the *quantization condition* for the energy E:

$$k(E)\tan(k(E)a/2) = \kappa(E)$$

Or, equivalently:

$$\tan\left(\frac{\sqrt{2mE}\,a}{2\hbar}\right) = \sqrt{\frac{V_0 - E}{E}} \qquad [1]$$

To analyze this equation further, introduce dimensionless versions of the system energy and the barrier height. In particular, recall the ground state energy eigenvalue of a particle in an particle in an infinitely deep box of width *a*, namely $E_{gs}^{\infty} = \frac{\hbar^2\pi^2}{2ma^2}$. Then, let $\varepsilon \equiv E/E_{gs}^{\infty}$ and $v_0 = V_0/E_{gs}^{\infty}$.

Substituting into Eq. [1] gives the equivalent equation:

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

Eq. 2 can be solved "graphically", as shown in Fig. 2.

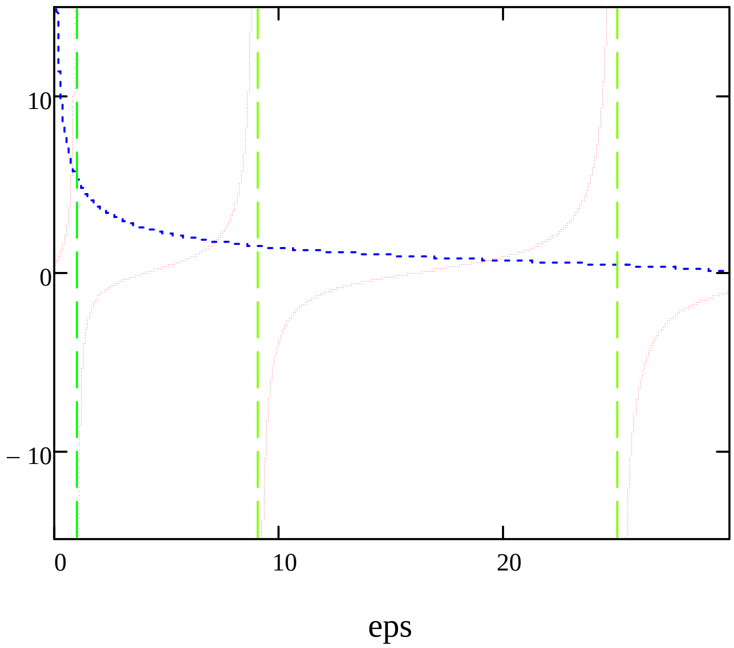


Fig. 2: For $v_0 = 30$, solid **red** line shows l.h.s. of Eq. 2; dotted **blue** line shows r.h.s. of Eq. 2. Dashed (vertical) **green** line shows locations of infinities of the l.h.s. of Eq. 2, corresponding to eps= ε =1,9,25,…

Precise determination of the intersection of the left and right hand sides of Eq. 2 (and hence the allowed values of $\varepsilon_1 = E_1 / E_{gs}^{\infty}$, etc.) requires [elementary] numerical analysis.

However, several qualitative features can be ascertained from the graphs in Fig. 2, including:

i) As $v_0 \to \infty$, the intersections come at $\varepsilon = 1, 9, 25$. These are precisely the even-parity energy levels (in units of E_{gs}^{∞}) of the infinite depth 1D Particle in a Box.

ii) There are only a finite number of solutions (crossings), i.e., a *finite* number of even-parity bound states in the box. [Of course, the odd-parity states need to be analyzed, too, but the same conclusion holds for these.]

iii) Each finite-depth PinB energy level is *lower* than the corresponding infinite-depth PinB level.

Plugging in numbers: If the particle is an electron ($m_e = 9.1\times 10^{-28}\,gm$) confined to a box of width $a = 10$ Å, then $E_{gs}^{\infty} \cong 0.38\,\mathrm{eV}$.

So, $v_0 = 30$ corresponds to a barrier height of 11.4 eV.

Furthermore, one finds numerically:

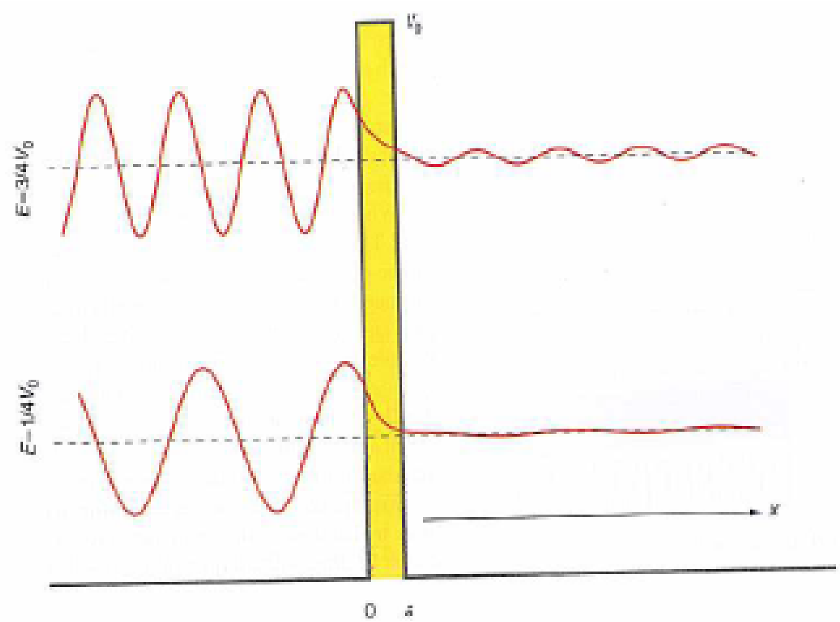
$\varepsilon_1 = 0.80$, or $E_1 = 0.31\,\mathrm{eV}$

$\varepsilon_2 = 7.2$, or $E_2 = 2.7$ eV

,etc.

Tunneling of a particle through a Barrier in 1D (see Engel Problem P5.6):

FIGURE 5.7
Waves corresponding to the indicated energy are incident from the left on a barrier of height $V_0 = 1.60 \times 10^{-19}$ J and width 9.00×10^{-10} m.



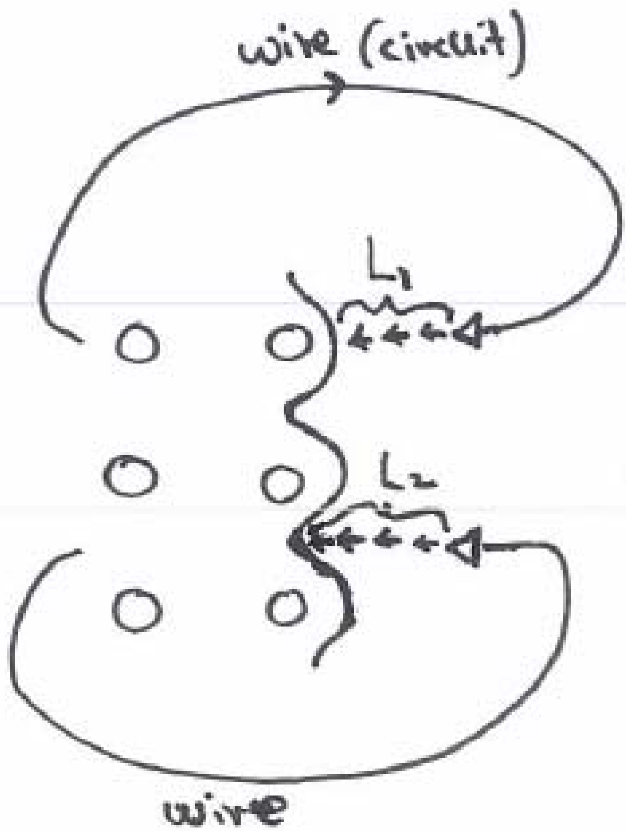
V_0 = 1.6 x 10^{-19} J.
a= 9 x 10^{-10} m

For a wide barrier , $\kappa a \gg 1$

Transmission Probability = $$\frac{16k^2\kappa^2 e^{-2\kappa a}}{(k^2+\kappa^2)^2}$$

with: $k = \sqrt{2mE}\,/\,\hbar$ $\quad\quad$ $\kappa = \sqrt{2m(V_0 - E)}\,/\,\hbar$

Underlying Principle of Scanning Tunneling Microscopy (STM):



Electrons tunnel between STM tip and atoms on a solid (metal) surface.

Some details of a Scanning Tunneling Microscope:

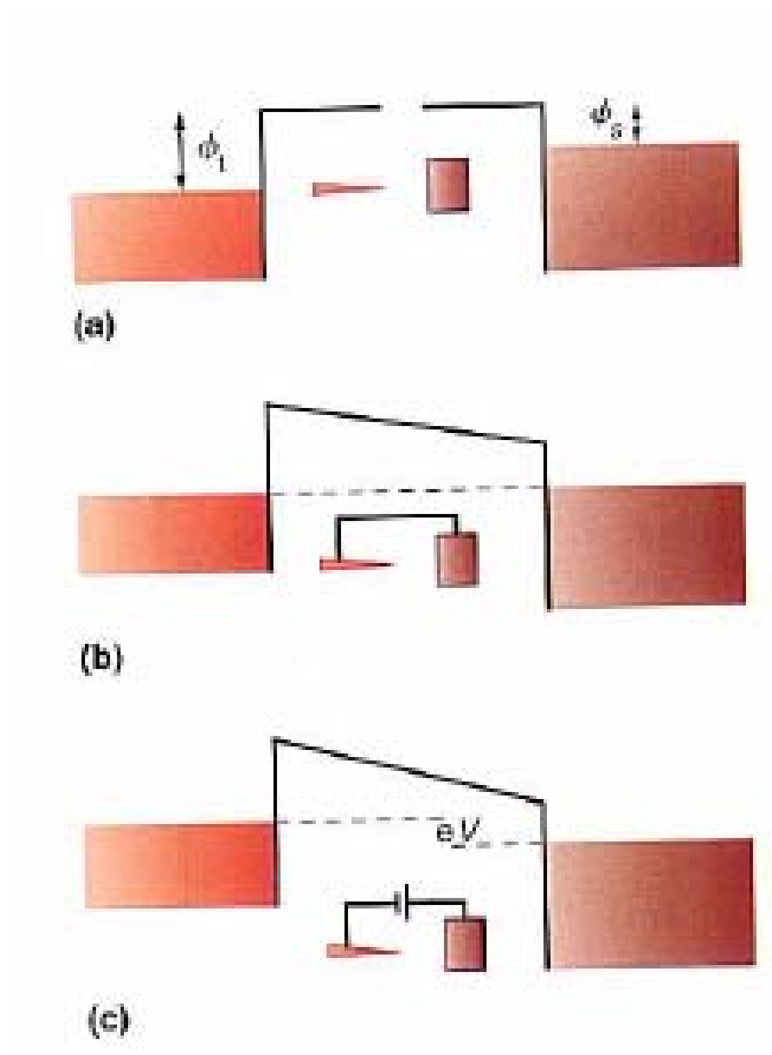


FIGURE 5.8
(a) If the conducting tip and surface are electrically isolated from one another, their energy diagrams line up. (b) If they are connected by a wire in an external circuit, charge flows from the lower work function material into the higher work function material until the highest occupied states have the same energy in both materials. (c) By applying a voltage V between the two materials, the highest occupied levels have an offset of energy eV. This allows tunneling to occur from left to right. The subscripts t and s refer to tip and surface.

Some STM images of the surface of Si:

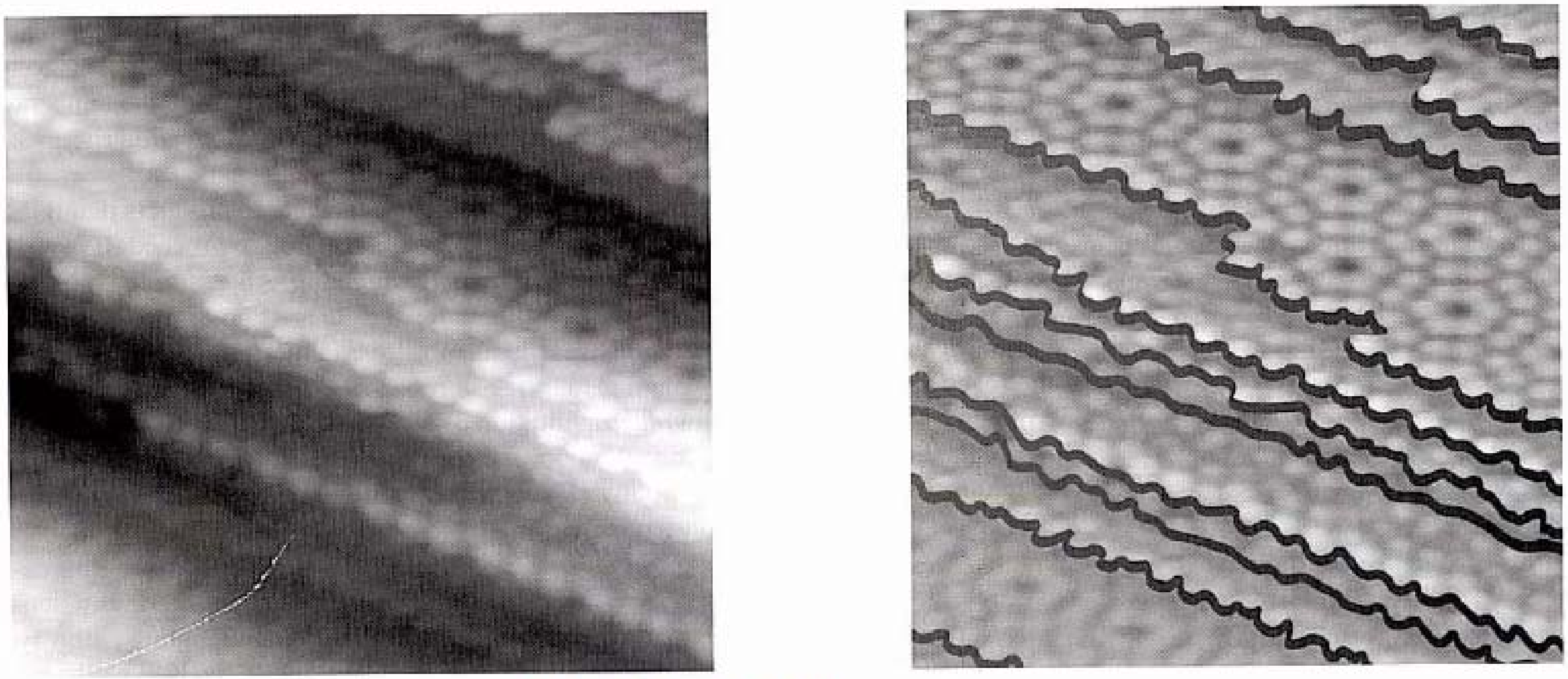


FIGURE 5.10

STM images of the (111) surface of Si. The left image shows a 200 × 200-nm region with a high density of atomic steps, and the light dots correspond to individual Si atoms. The right image shows how the image is related to the structure of parallel crystal planes separated by steps of one atom height. The step edges are shown as dark ribbons. [Courtesy of Kevin Johnson, University of Washington thesis, 1991.]