IV. 5 Scattering from a Square-Well Potential and a Square-Barrier Potential

A typical square-well potential is shown in Fig. IV.5.1.

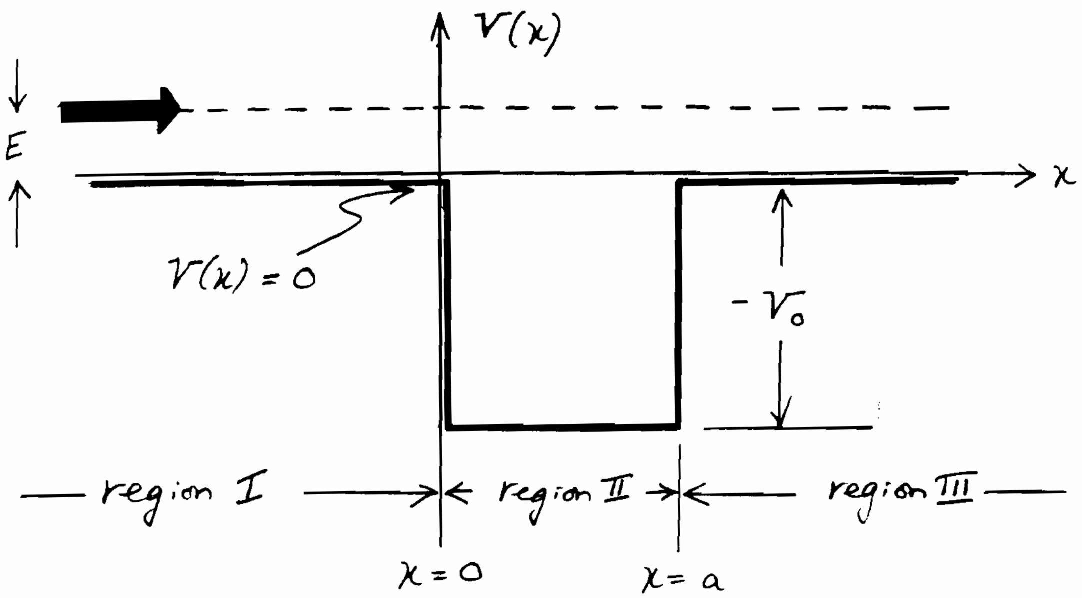


Fig. IV. 5.1. A square-well potential of depth V_0 and width a. The dashed line symbolizes the energies of particles in a beam incident from the left.

Again, we consider a beam of particles incident on the well from the left and the beam is analyzed as a steady-state problem.

With reference to Fig. IV. 5.1, the time-independent Schrödinger equation for region I is

$$\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x), \qquad (5.1)$$

for region II is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} - V_0\psi(x) = E\psi(x), \qquad (5.2)$$

and for region III is the same as region I. Equations (5.1) and (5.2) can be written in the form of eq. (2.3) and, thus, solutions for regions I, II and III can be written in the form of eq. (2.6); i.e.

for region I

$$\psi_I(x) = Ae^{ik_1x} + Be^{-ik_1x}, \qquad (5.3)$$

for region II

$$\psi_{II}(x) = Ce^{ik_2x} + De^{-ik_2x}, \qquad (5.4)$$

for region III (no beam from the right)

$$\psi_{III}(x) = Fe^{ik_1x}, \qquad (5.5)$$

where

$$k_1 = \sqrt{\frac{2mE}{\hbar^2}} \qquad (5.6)$$

and

$$k_2 = \sqrt{\frac{2m(E+V_0)}{\hbar^2}}; \qquad (5.7)$$

and A, B, C, D, and F are (complex) constants.

These solutions are required to obey the boundary conditions at $x = 0$ and $x = a$; i.e.

$$\psi_I(x=0) = \psi_{II}(x=0), \quad \psi_{II}(x=a) = \psi_{III}(x=a), \qquad (5.8)$$

$$\psi_I'(x)\Big|_{x=0} = \psi_{II}'(x)\Big|_{x=0}, \quad \psi_{II}'(x)\Big|_{x=a} = \psi_{III}'(x)\Big|_{x=a}. \qquad (5.9)$$

Thus,

$$A + B = C + D, \tag{5.10}$$

$$Ce^{ik_2a} + De^{-ik_2a} = Fe^{ik_1a}, \tag{5.11}$$

$$k_1A - k_1B = k_2C - k_2D, \tag{5.12}$$

and

$$k_2Ce^{ik_2a} - k_2De^{-ik_2a} = k_1Fe^{ik_1a}. \tag{5.13}$$

We are concerned with details of the reflected and transmitted beams which are described by the constants B and F, respectively. We proceed by eliminating C and D from eqs. (5.10) – (5.13). Multiplying eq. (5.11) by k_2 and adding to eq. (5.13),

$$2k_2Ce^{ik_2a} = (k_1+k_2)Fe^{ik_1a}, \tag{5.14}$$

$$\therefore \quad C = \frac{1}{2}\left(1+\frac{k_1}{k_2}\right)Fe^{i(k_1-k_2)a}. \tag{5.15}$$

Multiplying eq (5.11) by k_2 and subtracting eq. (15.13),

$$2k_2De^{-ik_2a} = (k_2-k_1)Fe^{ik_1a}, \tag{5.16}$$

$$\therefore \quad D = \frac{1}{2}\left(1-\frac{k_1}{k_2}\right)Fe^{i(k_1+k_2)a}. \tag{5.17}$$

Then, multiplying eq. (5.10) by k_1 and adding to eq. (5.12),

$$2k_1 A = (k_1 + k_2)C + (k_1 - k_2)D, \qquad (5.18)$$

and from eqs. (5.15) and (5.17),

$$\therefore A = \frac{1}{2k_1}\left\{(k_1+k_2)\frac{1}{2}\left(1+\frac{k_1}{k_2}\right)Fe^{i(k_1-k_2)a} + (k_1-k_2)\frac{1}{2}\left(1-\frac{k_1}{k_2}\right)Fe^{i(k_1+k_2)a}\right\}$$

$$= \frac{F}{4}e^{ik_1a}\left\{\left(2+\frac{k_2}{k_1}+\frac{k_1}{k_2}\right)e^{-ik_2a} + \left(2-\frac{k_2}{k_1}-\frac{k_1}{k_2}\right)e^{ik_2a}\right\}. \qquad (5.19)$$

Then using $e^{i\phi} = \cos\phi + i\sin\phi$

$$\therefore A = \frac{F}{4}e^{ik_1a}\left\{4\cos k_2a - 2i\left(\frac{k_2}{k_1}+\frac{k_1}{k_2}\right)\sin k_2a\right\}. \qquad (5.20)$$

The <u>transmission coefficient</u>, T is defined by

$$T \equiv \frac{\text{transmitted flux}}{\text{incident flux}} = \frac{|F|^2 k_1\hbar/m}{|A|^2 k_1\hbar/m} = \frac{|F|^2}{|A|^2}, \qquad (5.21)$$

whence

$$\frac{1}{T} = \frac{|A|^2}{|F|^2} = \left\{\cos^2 k_2a + \frac{1}{4}\left(\frac{k_2}{k_1}+\frac{k_1}{k_2}\right)^2\sin^2 k_2a\right\}$$

problem

$$= 1 + \left\{\frac{1}{4}\left(\frac{k_2^2+k_1^2}{k_1k_2}\right)^2 - 1\right\}\sin^2 k_2a$$

$$= 1 + \left\{\frac{k_2^4 + 2k_2^2k_1^2 + k_1^4 - 4k_1^2k_2^2}{4k_1^2k_2^2}\right\}\sin^2 k_2a. \qquad (5.22)$$

$$\therefore \frac{1}{T} = 1 + \frac{(k_2^2 - k_1^2)^2}{4k_1^2 k_2^2} \sin^2 k_2 a \,. \qquad (5.23)$$

Then, using eqs. (5.6) and (5.7)

$$\frac{1}{T} = 1 + \frac{(E + V_0 - E)^2}{4E(E + V_0)} \sin^2 k_2 a \,. \qquad (5.24)$$

$$\therefore \boxed{T = \frac{1}{1 + \frac{1}{4} \frac{V_0^2}{E(E+V_0)} \sin^2 k_2 a}} \,. \qquad (5.25)$$

Note that $T = 1$ if $\sin k_2 a = 0$, i.e. $k_2 a = n\pi$.
Hence, from eq. (5.7) if

$$E = \frac{n^2 h^2}{8 m a^2} - V_0 \,, \quad n \text{ integer}, \; E > 0 \qquad (5.26)$$

the beam is 100% transmitted. The conditions that fulfil $\sin k_2 a = 0$ are called <u>transmission resonances</u>.

A typical square-barrier potential is shown in Fig. IV. 5.2. The analysis of a beam of particles incident from the left on the barrier can be adapted directly from the analysis of the square-well potential by the simple replacement of $(E + V_0)$ by $(E - V_0)$ in region II and, in particular, in eqs. (5.7) and (5.25), i.e.

$$k_2 = \sqrt{\frac{2m(E - V_0)}{\hbar^2}} \,, \qquad (5.27)$$

$$\boxed{T = \frac{1}{1 + \frac{1}{4} \frac{V_0^2}{E(E-V_0)} \sin^2 k_2 a}} \,. \qquad (5.28)$$

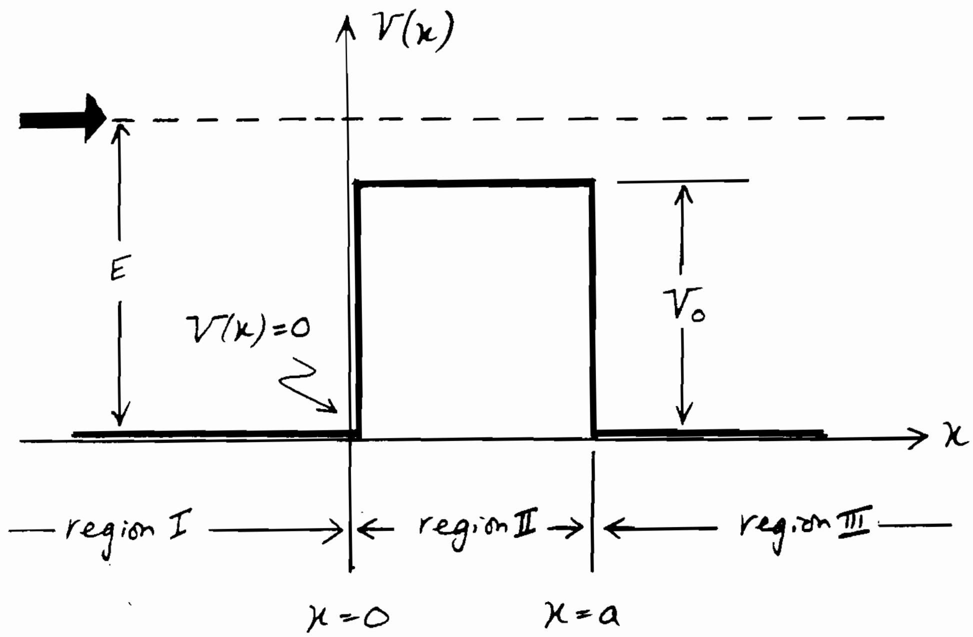
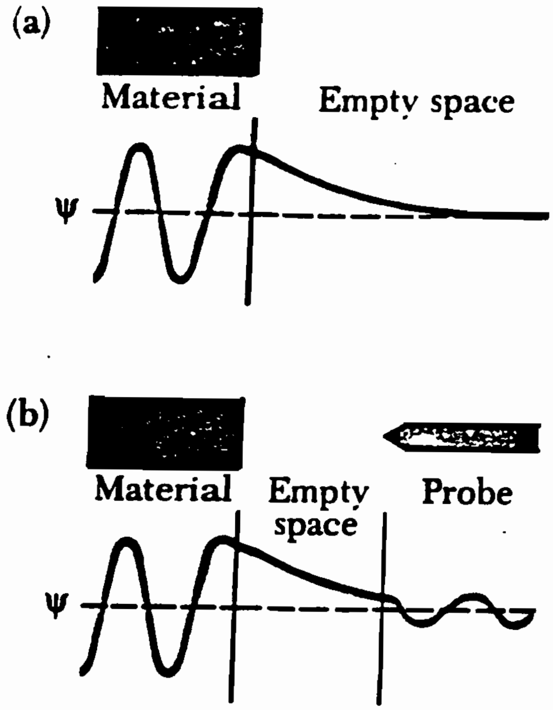
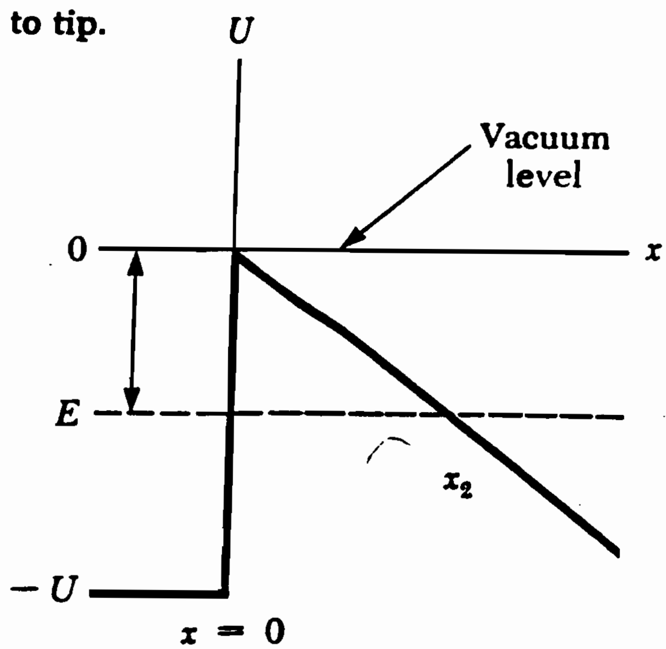


Fig. IV.5.2. A square-barrier potential of height V_0 and width a. Compare with Fig. IV.5.1.

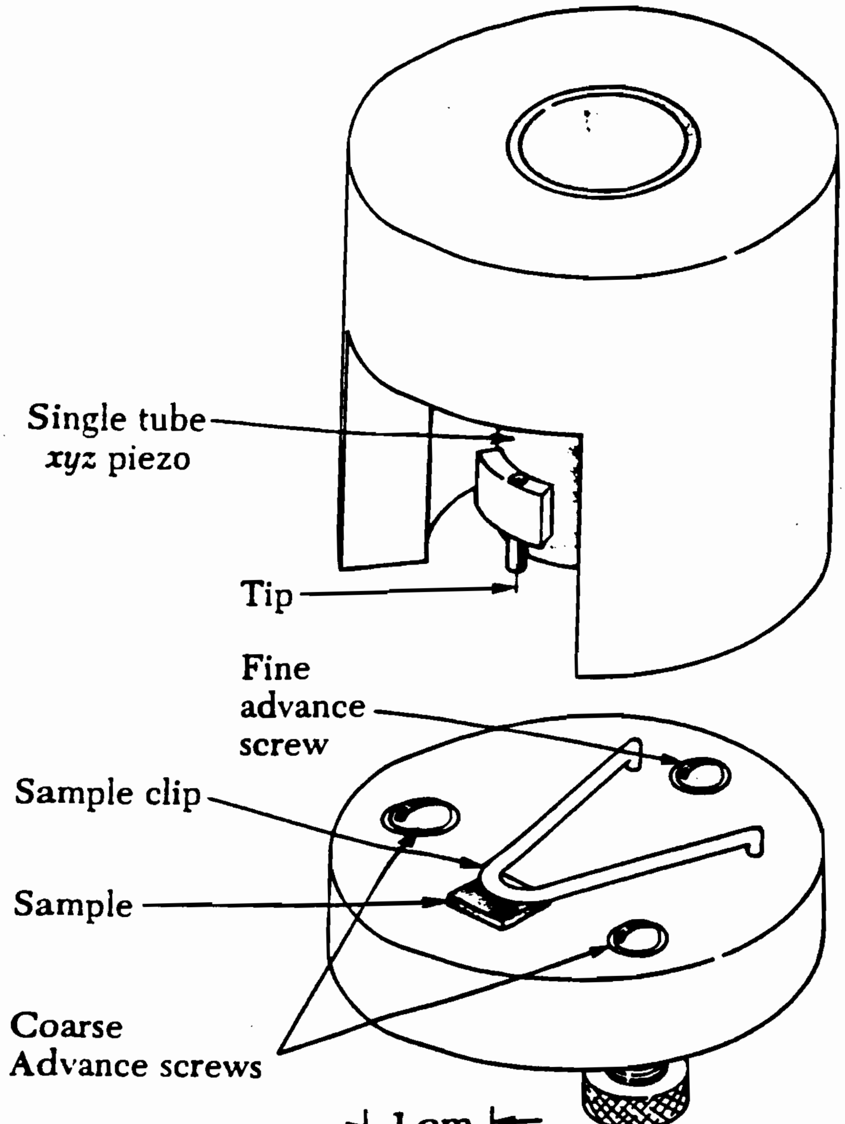
Scanning tunneling microscope image of the surface of crystalline gold. The divisions on the scale are 5 Å. Successive scans are approximately 1.5 Å apart. The figure is from G. Binning, H. Rohrer, Ch. Gerber, and E. Stoll, *Surface Science* 144:321, 1984.



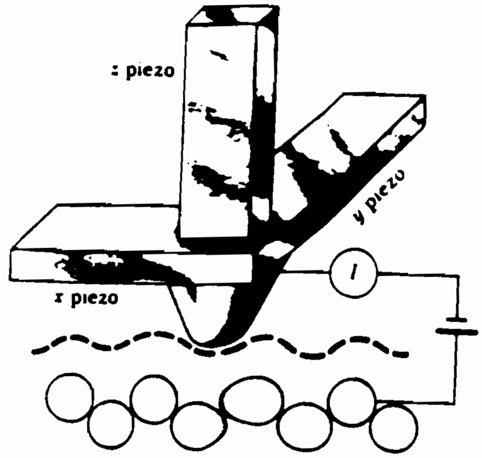
(a) The wave function of an electron in the surface of the material to be studied. The wave function extends beyond the surface into the empty region. (b) The sharp tip of a conducting probe is brought close to the surface. The wave function of a surface electron penetrates into the tip, so that the electron can "tunnel" from surface to tip.



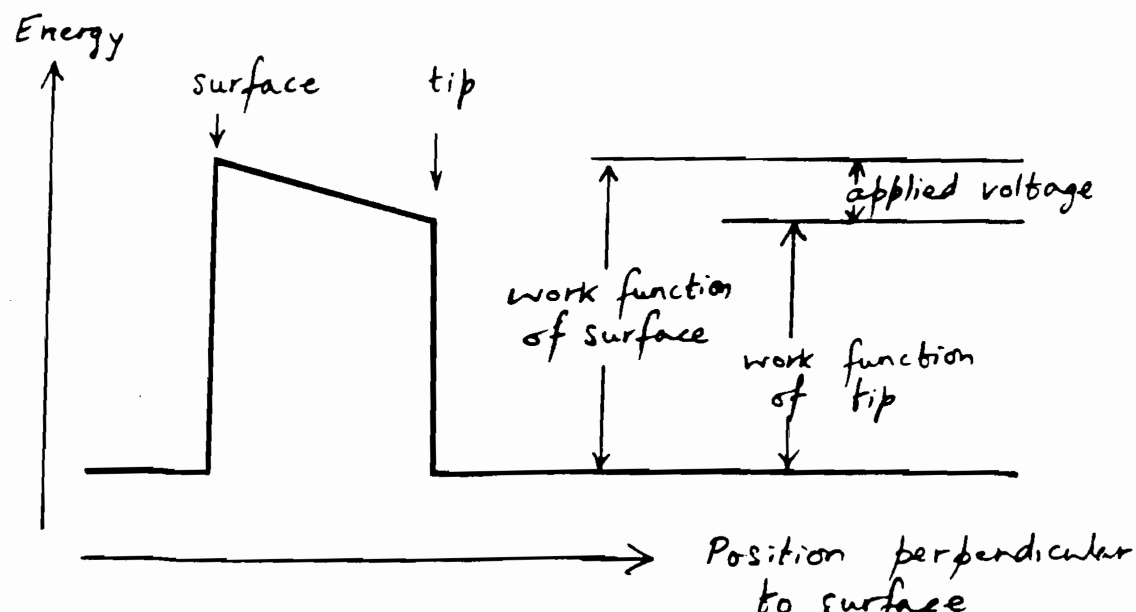
The potential energy versus position for an electron in a metal. The potential energy is $-U$ when the electron is in the metal ($x < 0$) and is proportional to x outside the metal ($x > 0$). An electron with energy E can escape the metal by tunneling from $x = 0$ to the point x_2.



Drawing of an actual STM head and base showing the essential components. Also depicted are the three screws used for controlling the mechanical approach of the tip to the sample. Three keys to a successful STM design are (1) A smooth mechanical approach mechanism, (2) rigidity, and (3) convenience in changing the sample and tip. (Based on a drawing from P.K. Hansma, V.B. Elings, O. Marti, and C.E. Bracker, *Science* 242:209–16, 1988. Copyright 1988 by the AAAS.)



A schematic view of an STM. The scanning tip is controlled by piezoelectric crystals. It is rastered over the surface to be analyzed such that the tunneling current between the surface and the tip is constant. The record of the z piezo movement is a profile of the surface, with atomic resolution.



A schematic view of the barrier (the gap between the surface and the scanning tip) through which electrons must tunnel. Typically, a small negative bias is put on the surface.