Quantum Mechanics I

PHY 3103

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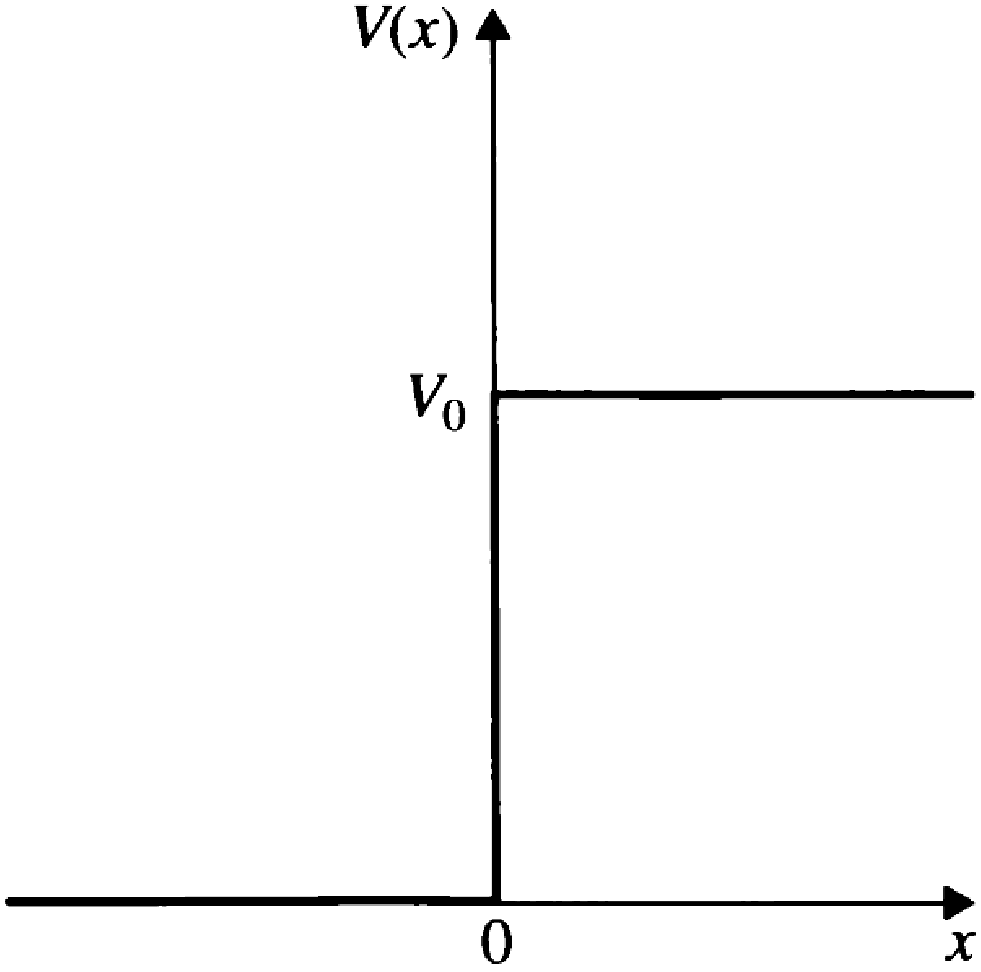
Potential Step

The potential step

$$V(x) = \begin{cases} 0, & x < 0, \\ V_0, & x \geq 0. \end{cases}$$

(a) Case $E > V_0$

(b) Case $E < V_0$



The potential step: (a) Case $E > V_0$

$$\left(\frac{d^2}{dx^2} + k_1^2\right)\psi_1(x) = 0 \qquad (x < 0)$$

$$\left(\frac{d^2}{dx^2} + k_2^2\right)\psi_2(x) = 0 \qquad (x \geq 0)$$

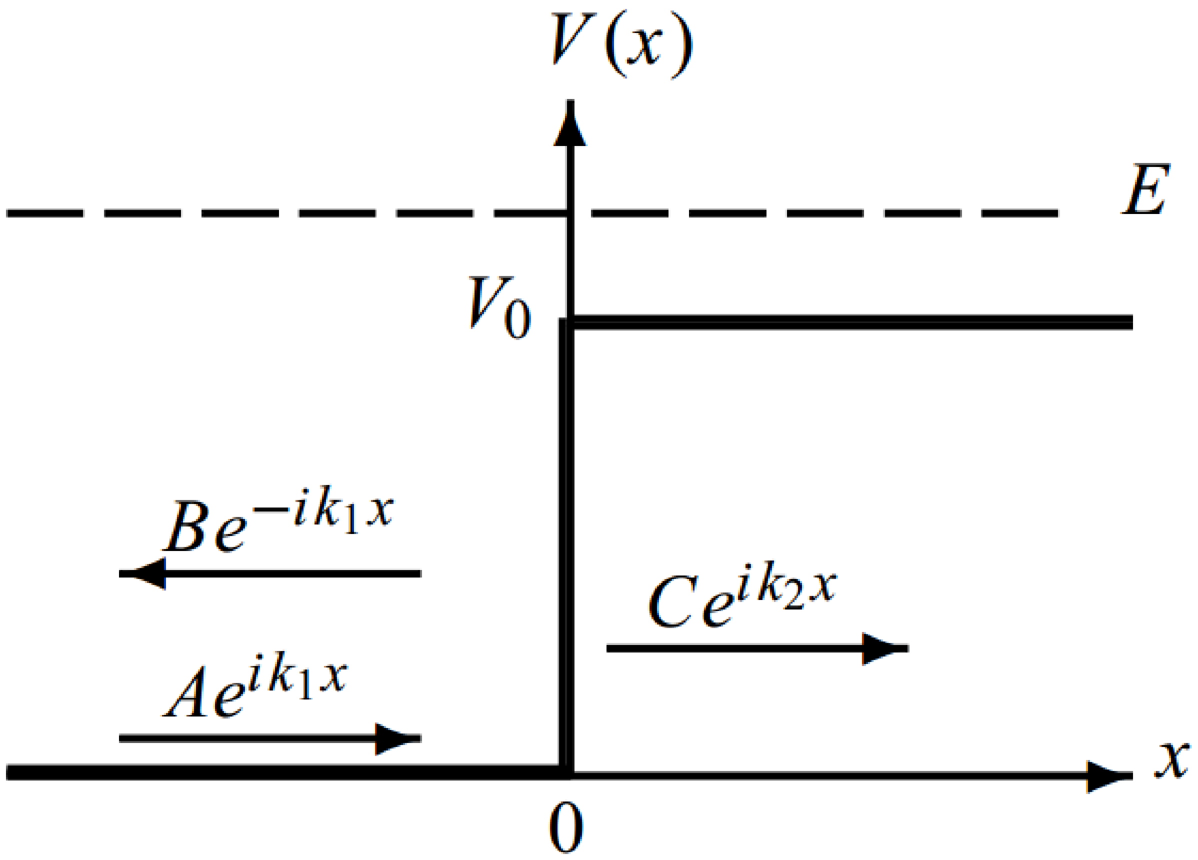
where $k_1^2 = 2mE/\hbar^2$

and $k_2^2 = 2m(E - V_0)/\hbar^2$.

The potential step: (a) Case $E > V_0$

$$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}$$

$$\psi_2(x) = Ce^{ik_2x}$$



The potential step: (a) Case $E > V_0$

The probability current density (probability flux)

$$j = \frac{\hbar}{2im}\left[\psi^*(x)\frac{d\psi(x)}{dx} - \psi(x)\frac{d\psi^*(x)}{dx}\right]$$

The potential step: (a) Case $E > V_0$

Let us now evaluate the *reflection* and *transmission coefficients*, *R* and *T*, as defined by

$$R = \left| \frac{\text{reflected current density}}{\text{incident current density}} \right| = \left| \frac{J_{reflected}}{J_{incident}} \right|$$

$$T = \left| \frac{J_{transmitted}}{J_{incident}} \right|$$

The potential step: (a) Case $E > V_0$

Since the incident wave is $\psi_i(x) = Ae^{ik_1 x}$,

$$J_{incident} = \frac{i\hbar}{2m}\left(\psi_i(x)\frac{d\psi_i^*(x)}{dx} - \psi_i^*(x)\frac{d\psi_i(x)}{dx}\right) = \frac{\hbar k_1}{m}|A|^2$$

The potential step: (a) Case $E > V_0$

Similarly, since the reflected and transmitted waves are

$\psi_r(x) = Be^{-ik_1x}$ and $\psi_t(x) = Ce^{ik_2x}$,

we can verify that the reflected and transmitted fluxes are

$$J_{reflected} = -\frac{\hbar k_1}{m}|B|^2, \qquad J_{transmitted} = \frac{\hbar k_2}{m}|C|^2.$$

The potential step: (a) Case $E > V_0$

$$R = \frac{|B|^2}{|A|^2}, \qquad T = \frac{k_2}{k_1}\frac{|C|^2}{|A|^2}$$

Thus, the calculation of R and T is reduced to determining the constants B and C . For this, we need to use the boundary conditions of the wave function at $x = 0$.

The potential step: (a) Case $E > V_0$

Since both the wave function and its first derivative are continuous at x = 0,

$$\psi_1(0) = \psi_2(0), \qquad \frac{d\psi_1(0)}{dx} = \frac{d\psi_2(0)}{dx},$$

$$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x} \qquad (x < 0)$$

$$\psi_2(x) = Ce^{ik_2x} \qquad (x \geq 0)$$

The potential step: (a) Case $E > V_0$

$$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x} \qquad (x < 0)$$

$$\psi_2(x) = Ce^{ik_2x} \qquad (x \geq 0)$$

$$A + B = C, \qquad k_1(A - B) = k_2C$$

$$B = \frac{k_1 - k_2}{k_1 + k_2}A, \qquad C = \frac{2k_1}{k_1 + k_2}A.$$

The potential step: (a) Case $E > V_0$

The constant A, it can be determined from the normalization condition of the wave function, but we don't need it here, since R and T are expressed in terms of ratios

$$R = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2} = \frac{(1 - \mathcal{K})^2}{(1 + \mathcal{K})^2}, \qquad T = \frac{4k_1 k_2}{(k_1 + k_2)^2} = \frac{4\mathcal{K}}{(1 + \mathcal{K})^2}$$

where $\mathcal{K} = k_2/k_1 = \sqrt{1 - V_0/E}$.

The sum of R and T is equal to 1, as it should be.

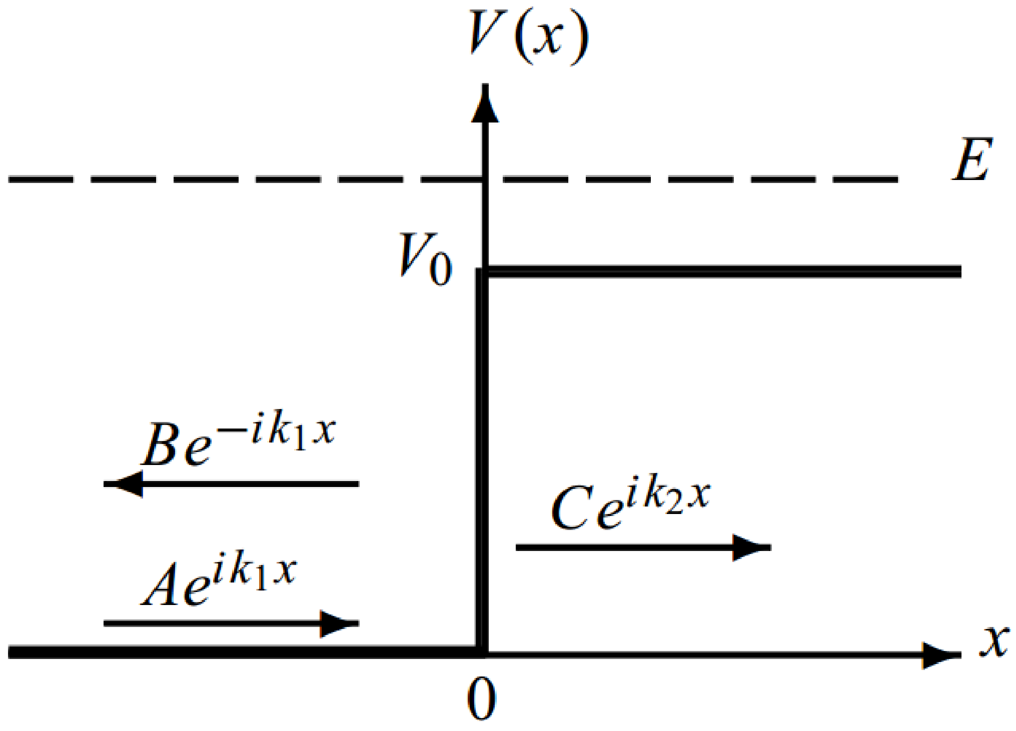
The potential step: (a) Case $E > V_0$

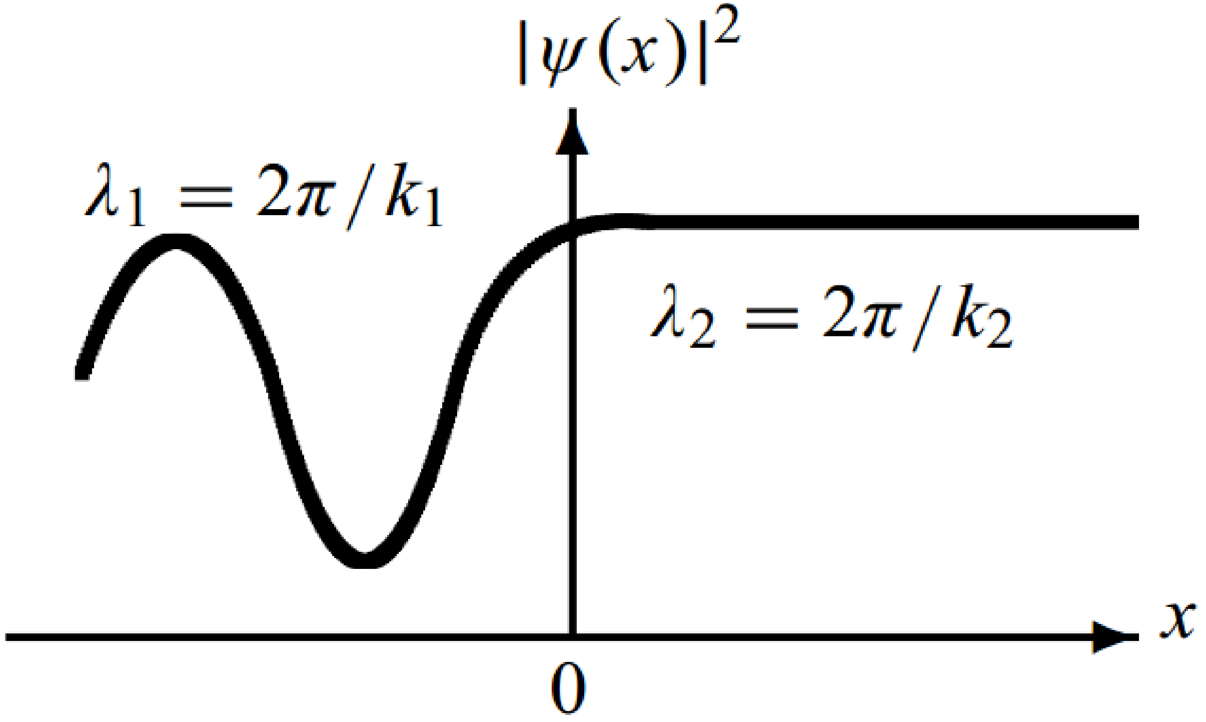
$$R = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2} = \frac{(1 - \mathcal{K})^2}{(1 + \mathcal{K})^2}, \qquad T = \frac{4k_1 k_2}{(k_1 + k_2)^2} = \frac{4\mathcal{K}}{(1 + \mathcal{K})^2}$$

where $\mathcal{K} = k_2/k_1 = \sqrt{1 - V_0/E}$.

As E gets smaller and smaller, T also gets smaller and smaller so that when $E = V_0$ the transmission coefficient T becomes zero and $R = 1$. On the other hand, when $E \gg V_0$, we have $\mathcal{K} = \sqrt{1 - V_0/E} \simeq 1$; hence $R = 0$ and $T = 1$.

The potential step: (a) Case $E > V_0$



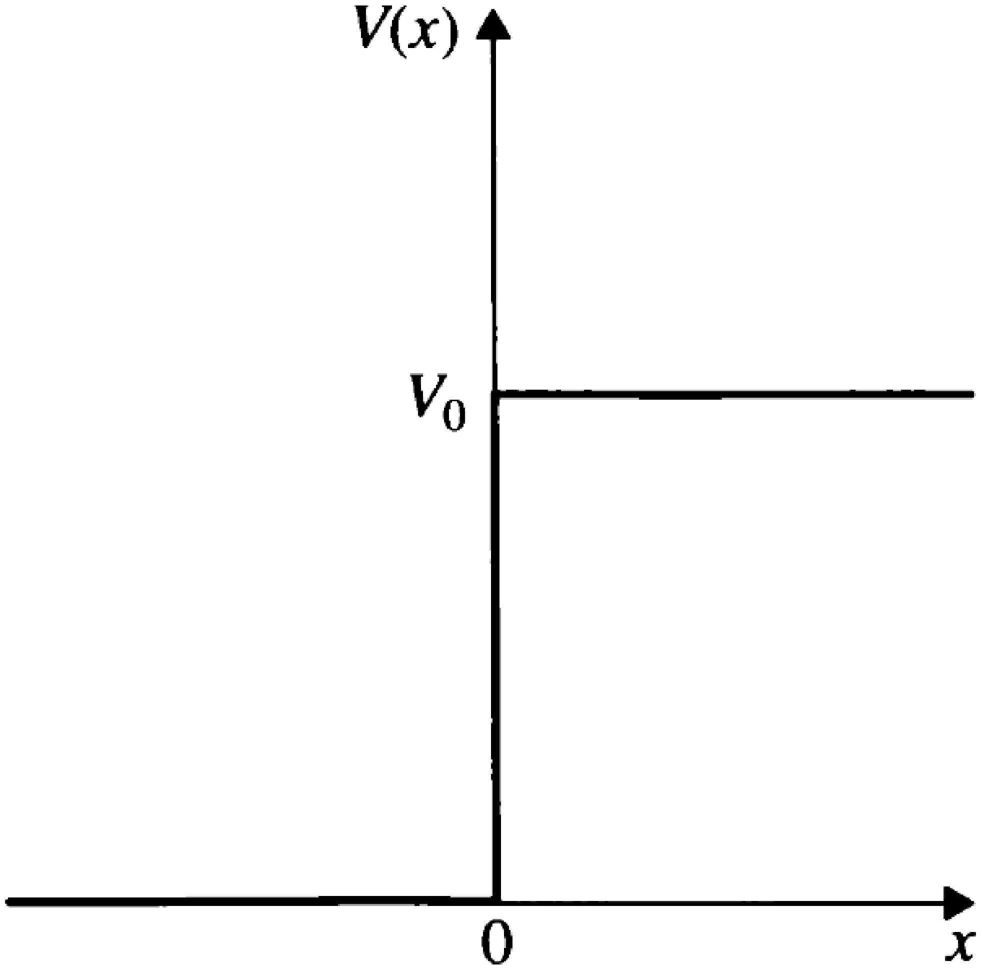


The potential step

$$V(x) = \begin{cases} 0, & x < 0, \\ V_0, & x \geq 0. \end{cases}$$

(a) Case $E > V_0$

(b) Case $E < V_0$



The potential step: (b) Case $E < V_0$

Classically, the particles arriving at the potential step from the left (with momenta $p = \sqrt{2mE}$) will come to a stop at $x = 0$ and then all will bounce back to the left with the magnitudes of their momenta unchanged. None of the particles will make it into the right side of the barrier $x = 0$; there is total reflection of the particles. So the motion of the particles is reversed by the potential barrier.

Quantum mechanically, the picture will be somewhat different.

The potential step: (b) Case $E < V_0$

$$\left(\frac{d^2}{dx^2} + k_1^2\right)\psi_1(x) = 0 \qquad (x < 0)$$

$$\left(\frac{d^2}{dx^2} - {k_2'}^2\right)\psi_2(x) = 0 \qquad (x \geq 0),$$

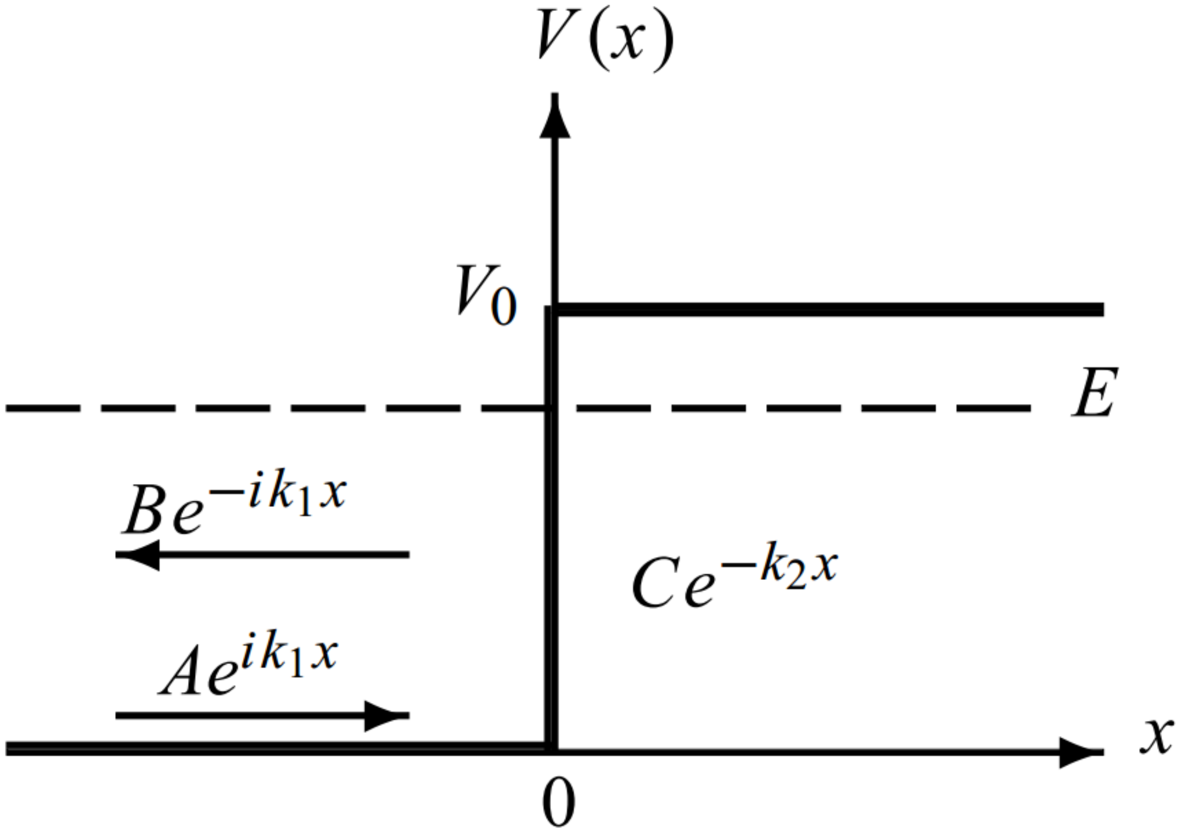
where $k_1^2 = 2mE/\hbar^2$

$${k_2'}^2 = 2m(V_0 - E)/\hbar^2.$$

The potential step: (b) Case $E < V_0$

$$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}$$

$$\psi_2(x) = Ce^{-k_2'x}$$



$$J_{transmitted} = \frac{\hbar}{2im}\left(\psi_t(x)\frac{d\psi_t(x)}{dx} - \psi_t(x)\frac{d\psi_t(x)}{dx}\right) = 0.$$

The potential step: (b) Case $E < V_0$

We can obtain

$$B = \frac{k_1 - ik_2'}{k_1 + ik_2'} A, \qquad C = \frac{2k_1}{k_1 + ik_2'} A$$

Thus, the reflected coefficient is given by

$$R = \frac{|B|^2}{|A|^2} = \frac{k_1^2 + k_2'^2}{k_1^2 + k_2'^2} = 1.$$

Total reflection, as in the classical case

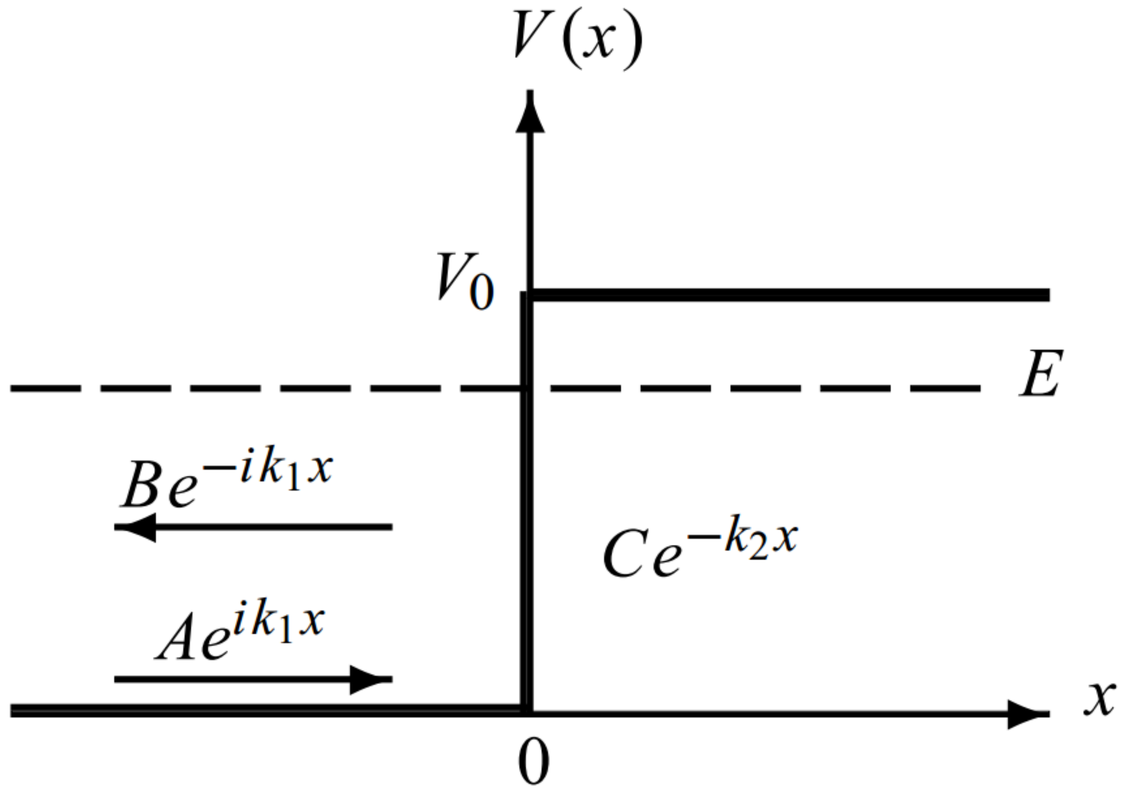
The potential step: (b) Case $E < V_0$

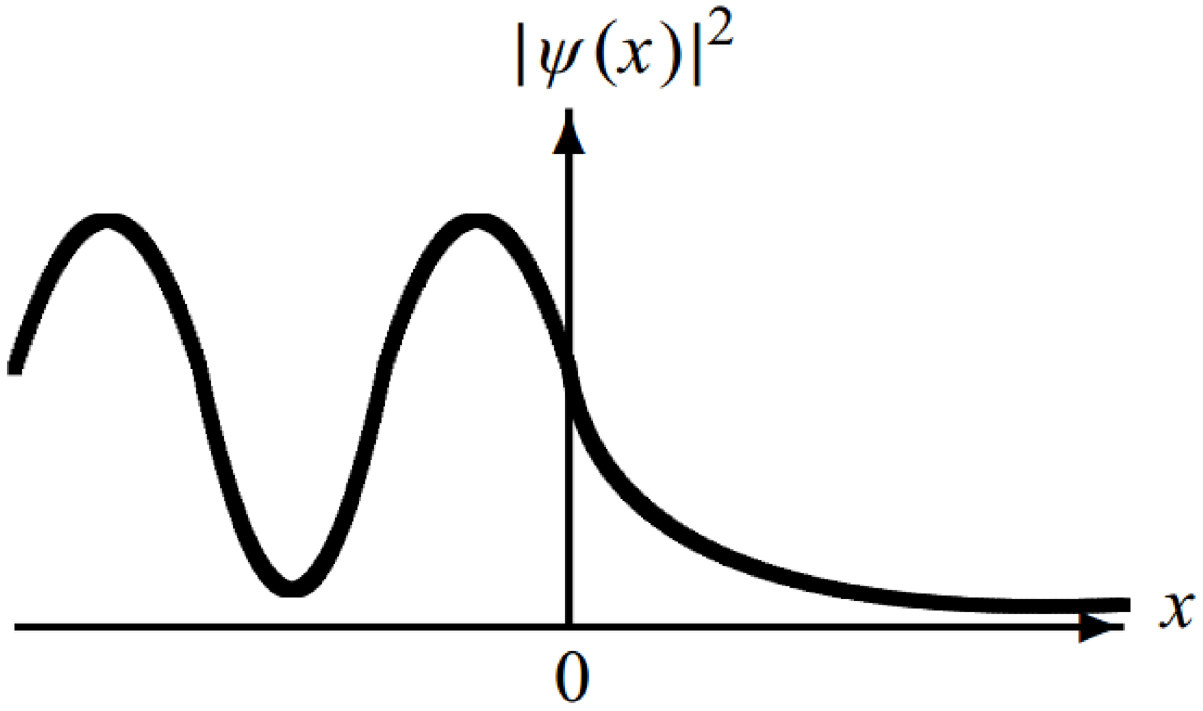
There is, however, a difference with the classical case: while none of the particles can be found classically in the region $x > 0$, quantum mechanically there is a nonzero probability that the wave function penetrates this classically forbidden region. To see this, note that the relative probability density

$$P(x) = |\psi_t(x)|^2 = |C|^2 e^{-2k_2' x} = \frac{4k_1^2 |A|^2}{k_1^2 + k_2'^2} e^{-2k_2' x}$$

is appreciable near $x = 0$ and falls exponentially to small values as x becomes large.

The potential step: (b) Case $E < V_0$

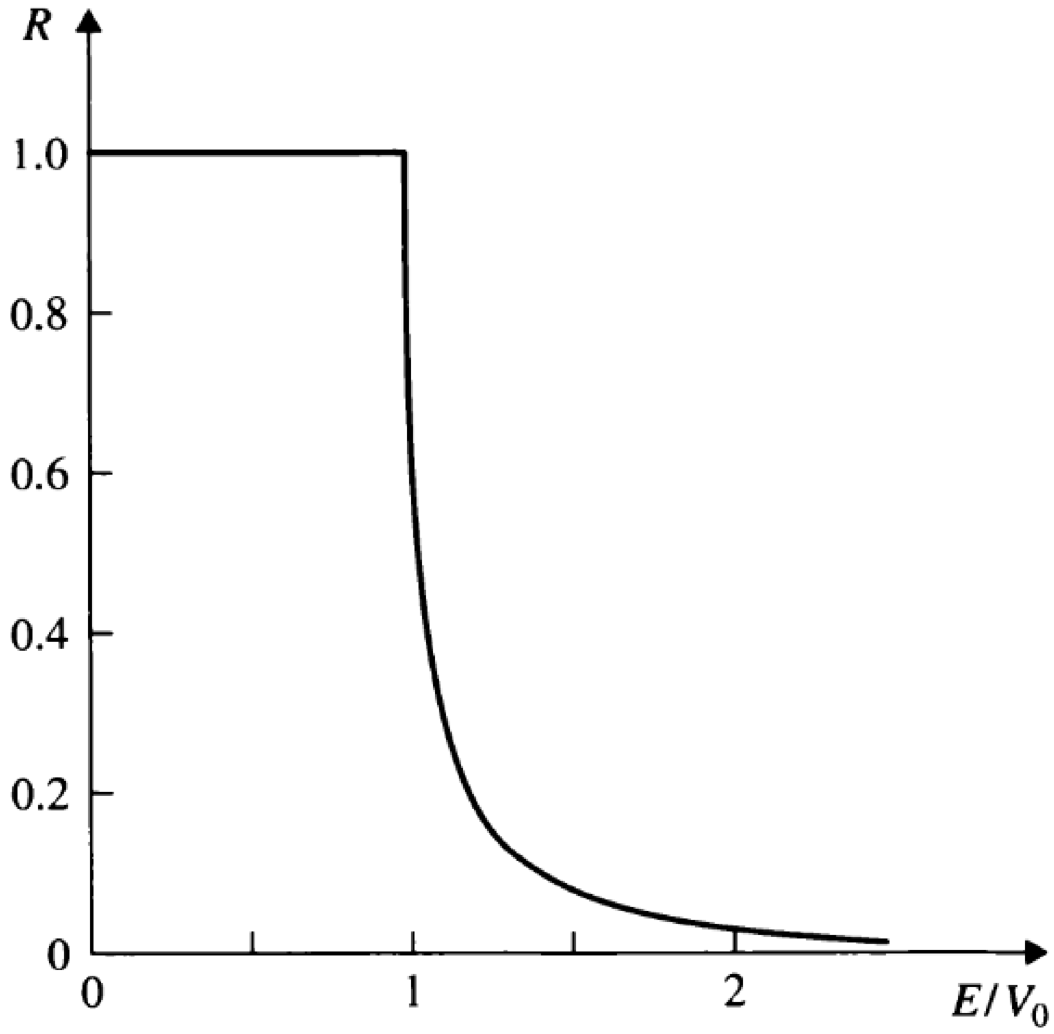




The potential step

$R = 1$ when $E = V_0$

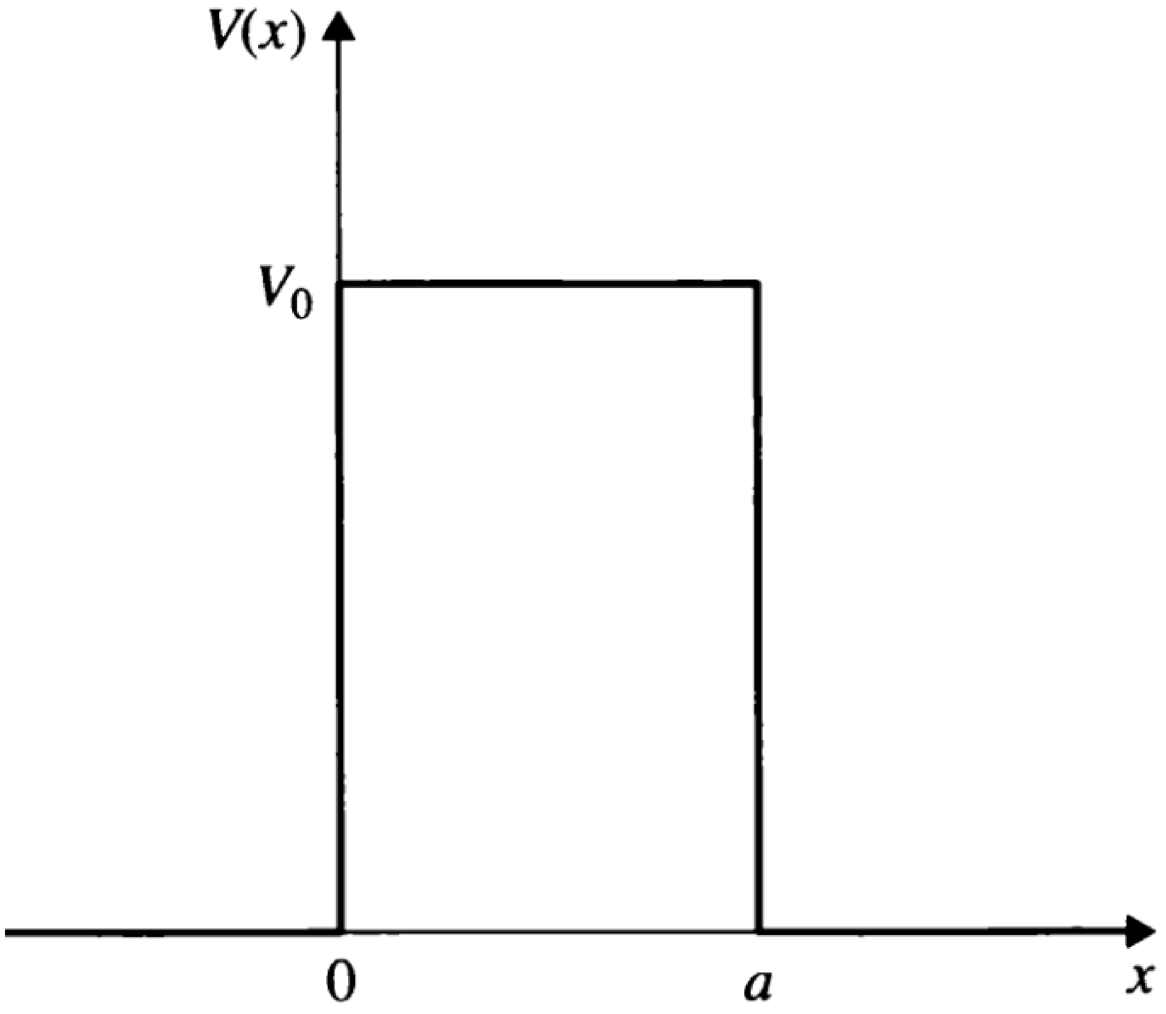
$R = 0$ when $E/V_0 \rightarrow \infty$



Tunnelling through a Potential Barrier

The potential barrier

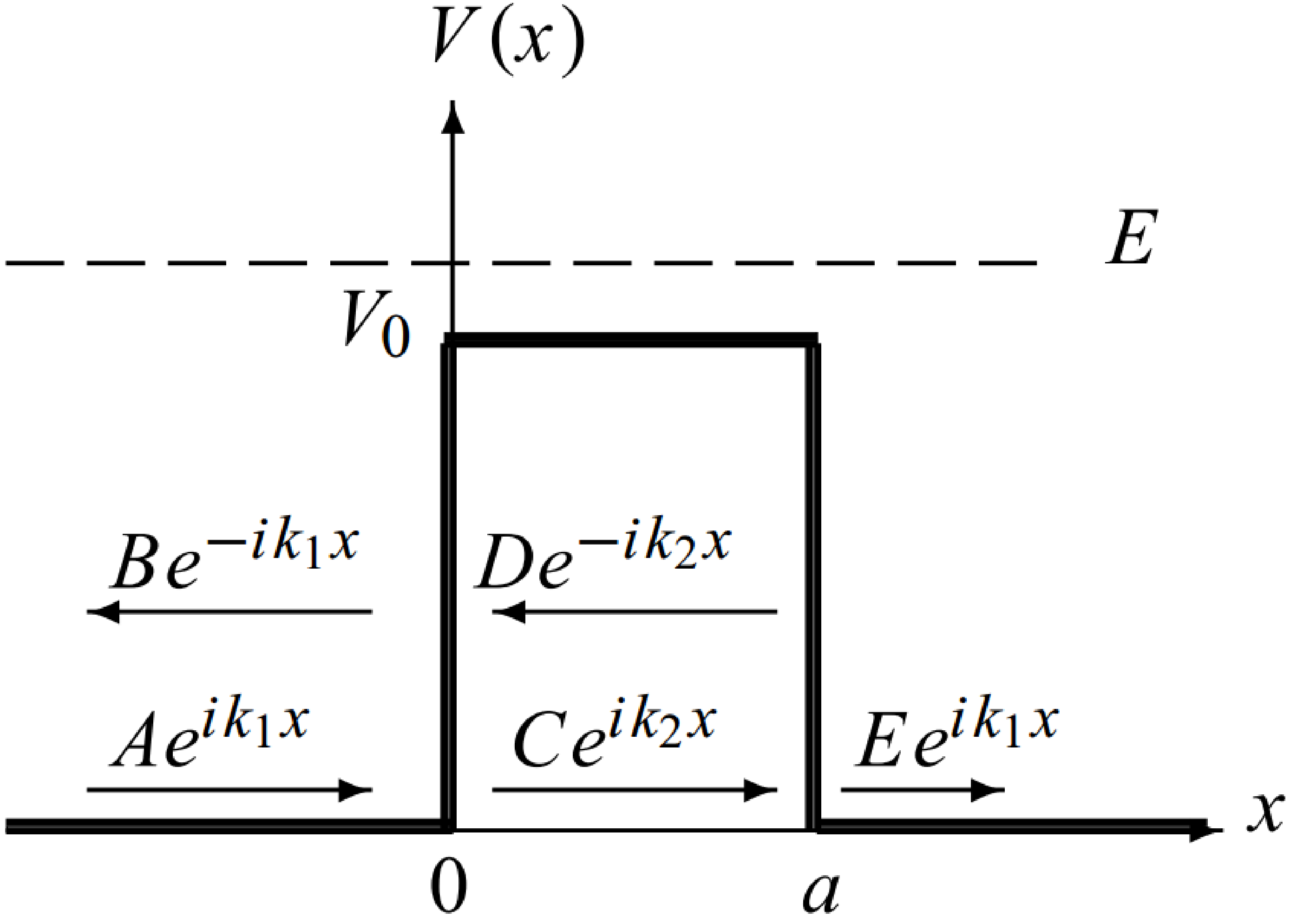
$$V(x) = \begin{cases} 0, & x < 0, \\ V_0, & 0 \le x \le a, \\ 0, & x > a. \end{cases}$$

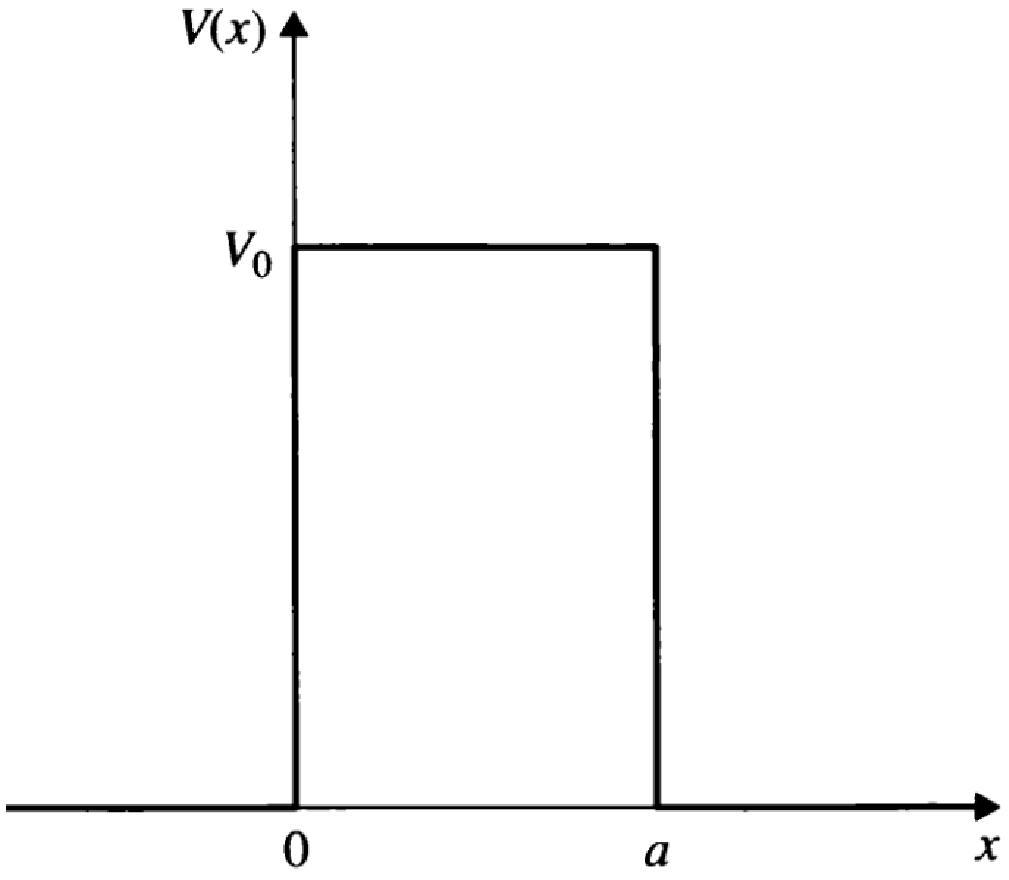


(a) Case $E > V_0$

(b) Case $E < V_0$

The potential barrier: (a) Case $E > V_0$



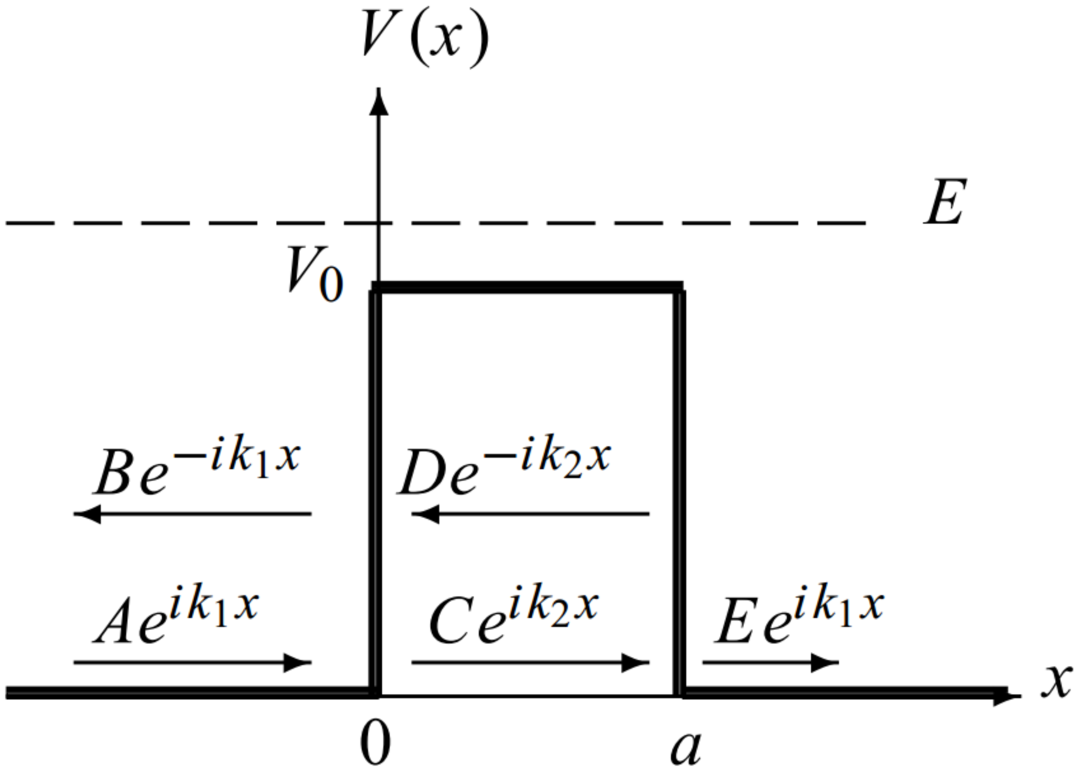


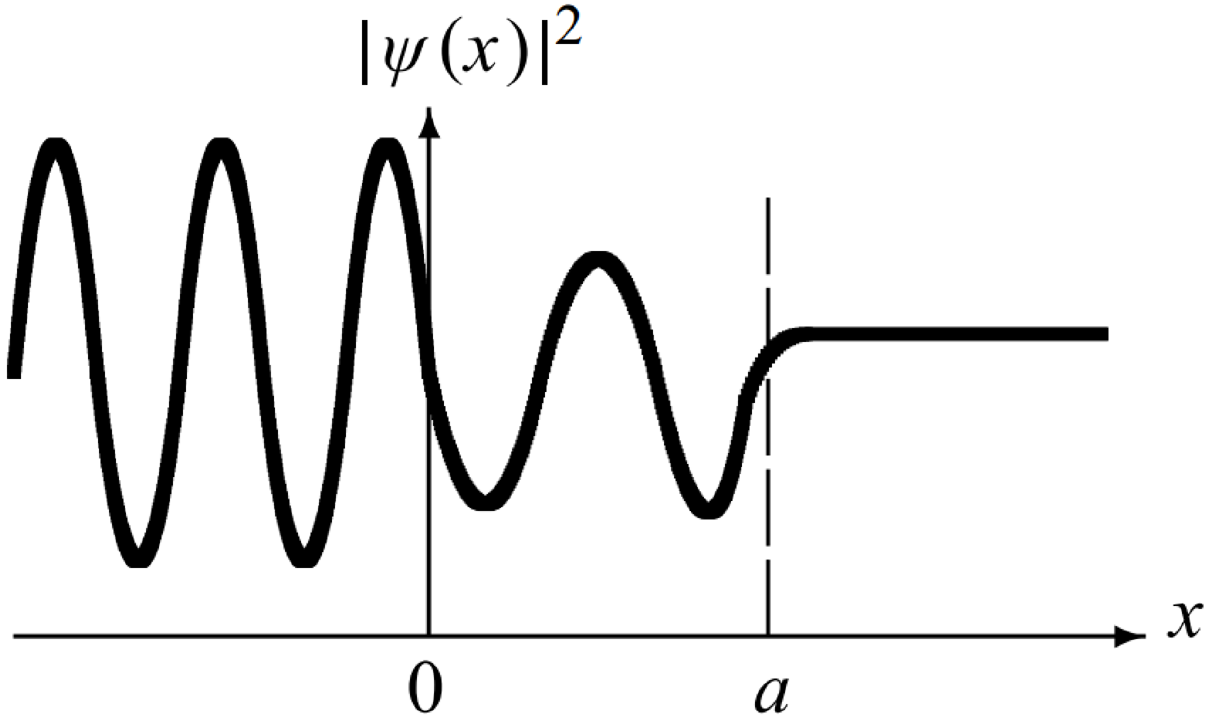
The potential barrier: (a) Case $E > V_0$

$$\psi(x) = \begin{cases} \psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}, & x \leq 0, \\ \psi_2(x) = Ce^{ik_2x} + De^{-ik_2x}, & 0 < x < a, \\ \psi_3(x) = Ee^{ik_1x}, & x \geq a, \end{cases}$$

where $k_1 = \sqrt{2mE/\hbar^2}$ and $k_2 = \sqrt{2m(E - V_0)/\hbar^2}$.

The potential barrier: (a) Case $E > V_0$





$E > V_0$

The potential barrier: (a) Case $E > V_0$

The constants *B*, *C*, *D*, and *E* can be obtained in terms of *A* from the boundary conditions: $\psi(x)$ and $d\psi/dx$ must be continuous at *x* = 0 and *x* =*a*, respectively:

$$\psi_1(0) = \psi_2(0), \qquad \frac{d\psi_1(0)}{dx} = \frac{d\psi_2(0)}{dx},$$

$$\psi_2(a) = \psi_3(a), \qquad \frac{d\psi_2(a)}{dx} = \frac{d\psi_3(a)}{dx}.$$

The potential barrier: (a) Case $E > V_0$

$$A + B = C + D, \qquad ik_1(A - B) = ik_2(C - D),$$

$$Ce^{ik_2a} + De^{-ik_2a} = Ee^{ik_1a}, \qquad ik_2\left(Ce^{ik_2a} - De^{-ik_2a}\right) = ik_1Ee^{ik_1a}.$$

Solving for E, we obtain

$$\begin{aligned} E &= 4k_1k_2Ae^{-ik_1a}\left[(k_1 + k_2)^2 e^{-ik_2a} - (k_1 - k_2)^2 e^{ik_2a}\right]^{-1} \\ &= 4k_1k_2Ae^{-ik_1a}\left[4k_1k_2\cos(k_2a) - 2i\left(k_1^2 + k_2^2\right)\sin(k_2a)\right]^{-1} \end{aligned}$$

The potential barrier: (a) Case $E > V_0$

The transmission coefficient is thus given by

$$T = \frac{k_1|E|^2}{k_1|A|^2} = \left[1 + \frac{1}{4}\left(\frac{k_1^2 - k_2^2}{k_1 k_2}\right)^2 \sin^2(k_2 a)\right]^{-1}$$

$$\left(\frac{k_1^2 - k_2^2}{k_1 k_2}\right)^2 = \frac{V_0^2}{E(E - V_0)}$$

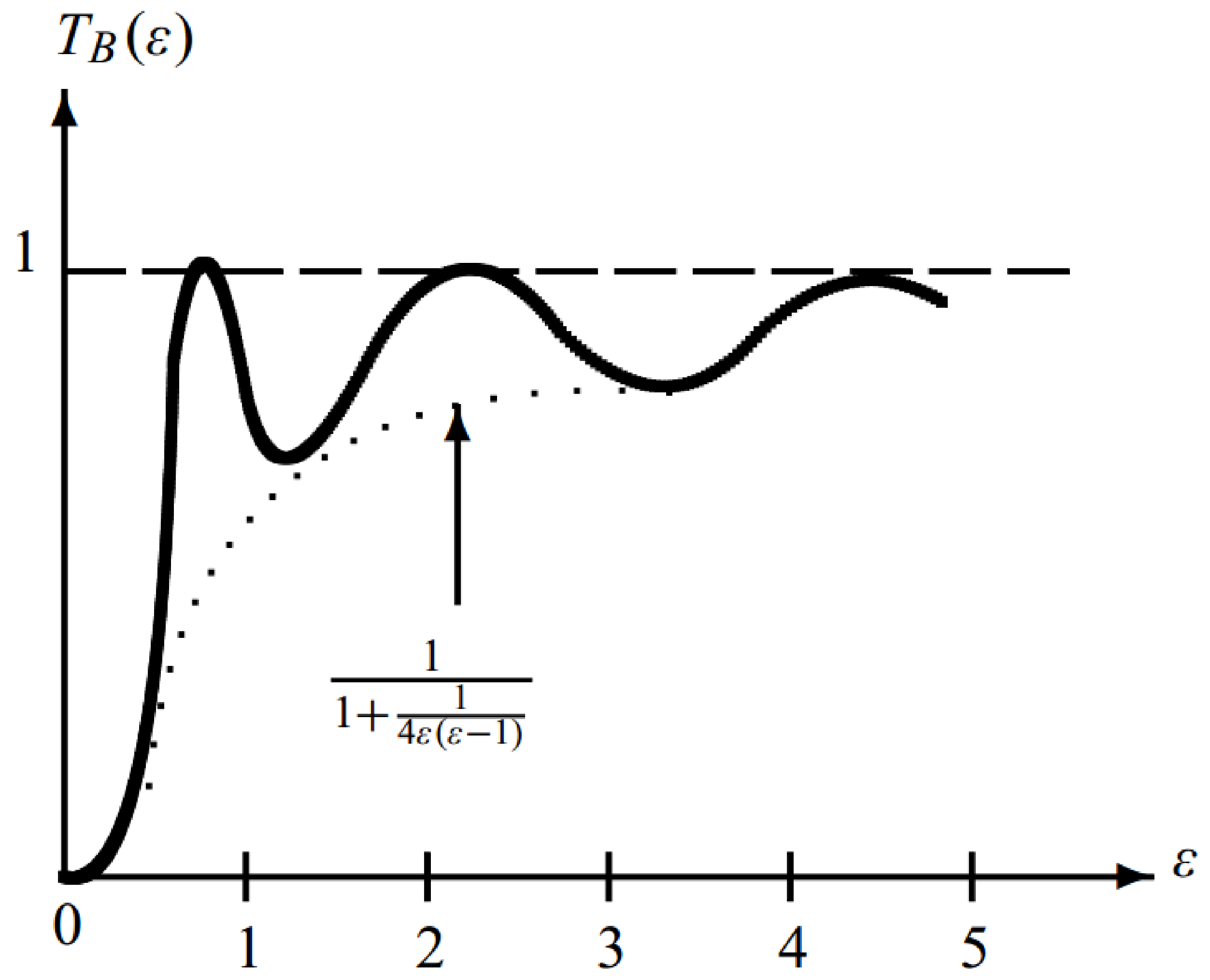
$$\lambda = a\sqrt{2mV_0/\hbar^2} \text{ and } \varepsilon = E/V_0$$

The potential barrier: (a) Case $E > V_0$

$$T = \left[1 + \frac{1}{4\varepsilon(\varepsilon - 1)} \sin^2\left(\lambda\sqrt{\varepsilon - 1}\right) \right]^{-1}$$

$$R = \frac{\sin^2\left(\lambda\sqrt{\varepsilon - 1}\right)}{4\varepsilon(\varepsilon - 1) + \sin^2\left(\lambda\sqrt{\varepsilon - 1}\right)} = \left[1 + \frac{4\varepsilon(\varepsilon - 1)}{\sin^2\left(\lambda\sqrt{\varepsilon - 1}\right)} \right]^{-1}$$

The potential barrier: (a) Case $E > V_0$



The potential barrier: (a) Case $E > V_0$

Special cases

- If $E \gg V_0$, and hence $\varepsilon \gg 1$, the transmission coefficient T becomes asymptotically equal to unity, $T \simeq 1$, and $R \simeq 0$. So, at very high energies and weak potential barrier, the particles would not feel the effect of the barrier; we have total transmission.

- In the limit $\varepsilon \to 1$ we have $\sin(\lambda\sqrt{\varepsilon - 1}) \sim \lambda\sqrt{\varepsilon - 1}$, hence (4.44) and (4.45) become

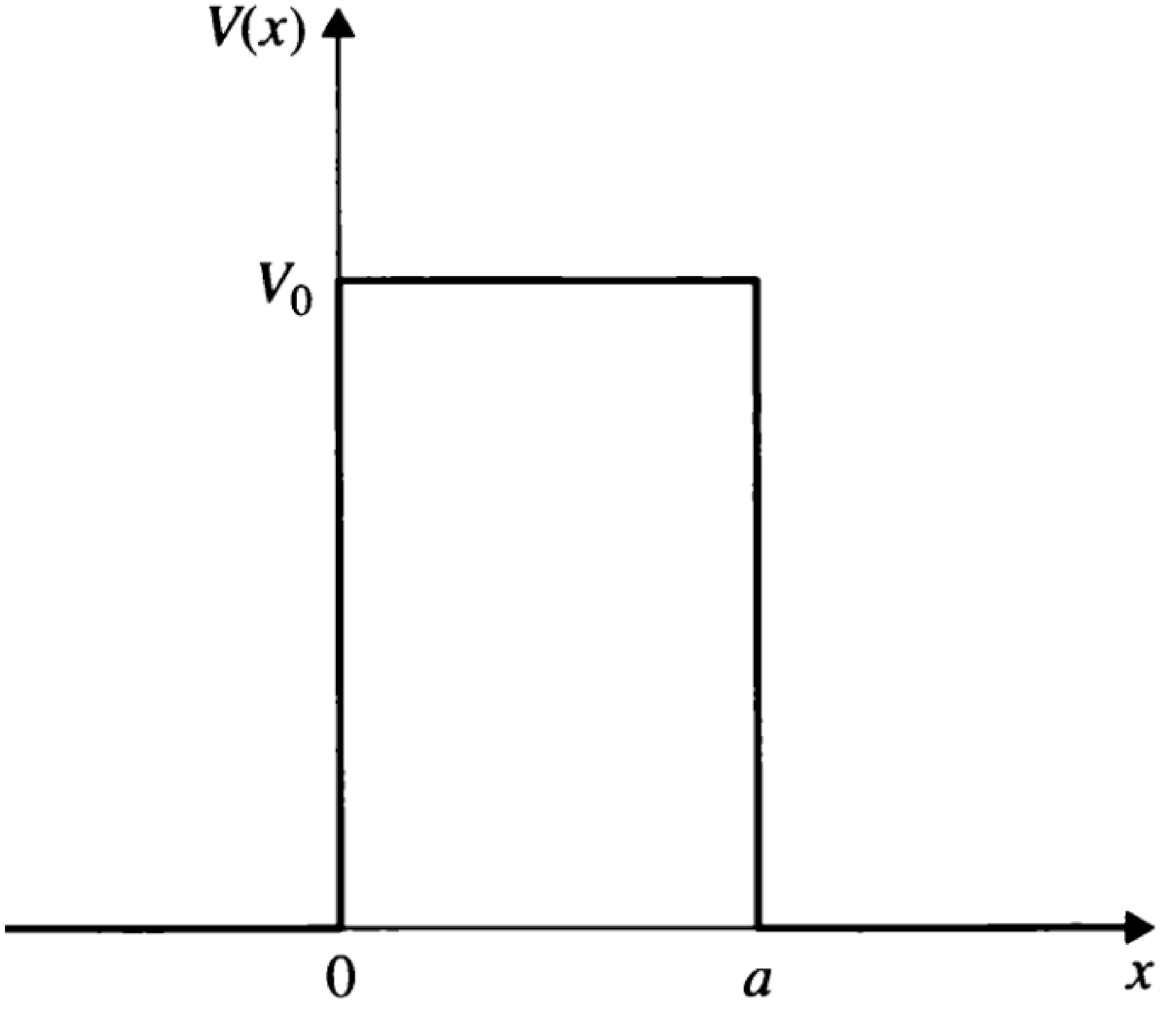
$$T = \left(1 + \frac{ma^2 V_0}{2\hbar^2}\right)^{-1}, \qquad R = \left(1 + \frac{2\hbar^2}{ma^2 V_0}\right)^{-1}.$$

The potential barrier

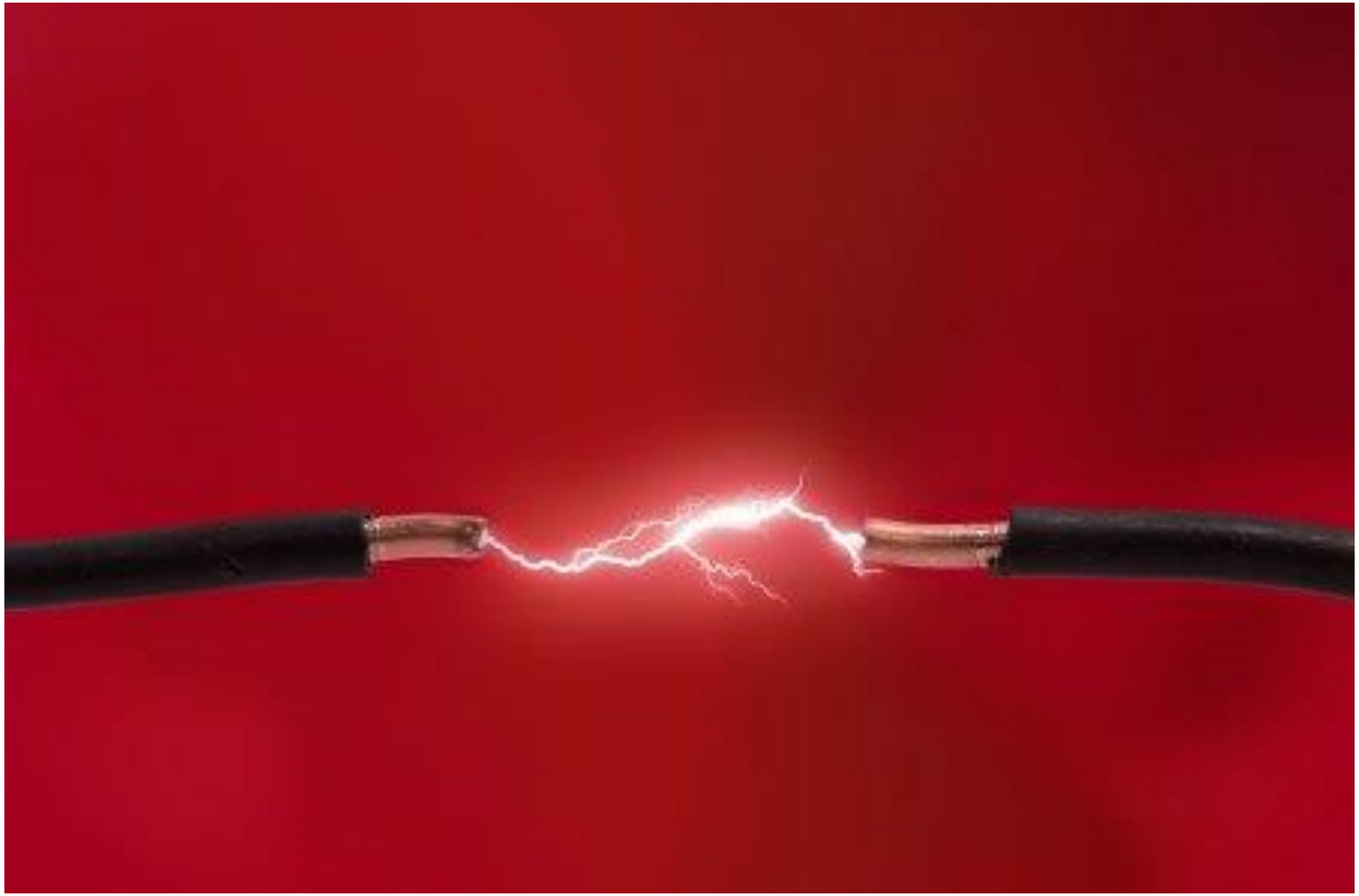
$$V(x) = \begin{cases} 0, & x < 0, \\ V_0, & 0 \le x \le a, \\ 0, & x > a. \end{cases}$$

(a) Case $E > V_0$

(b) Case $E < V_0$



The potential barrier

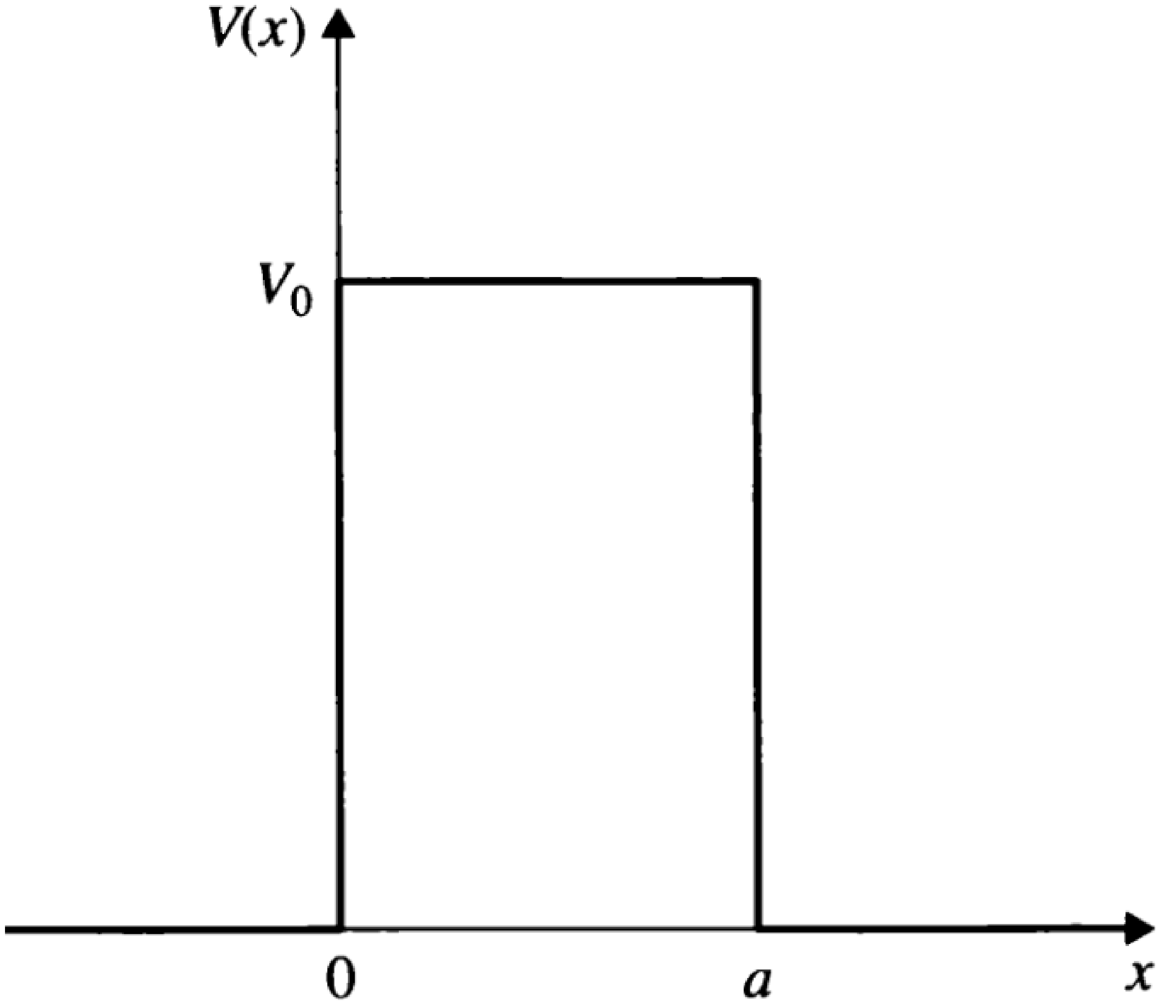


The potential barrier

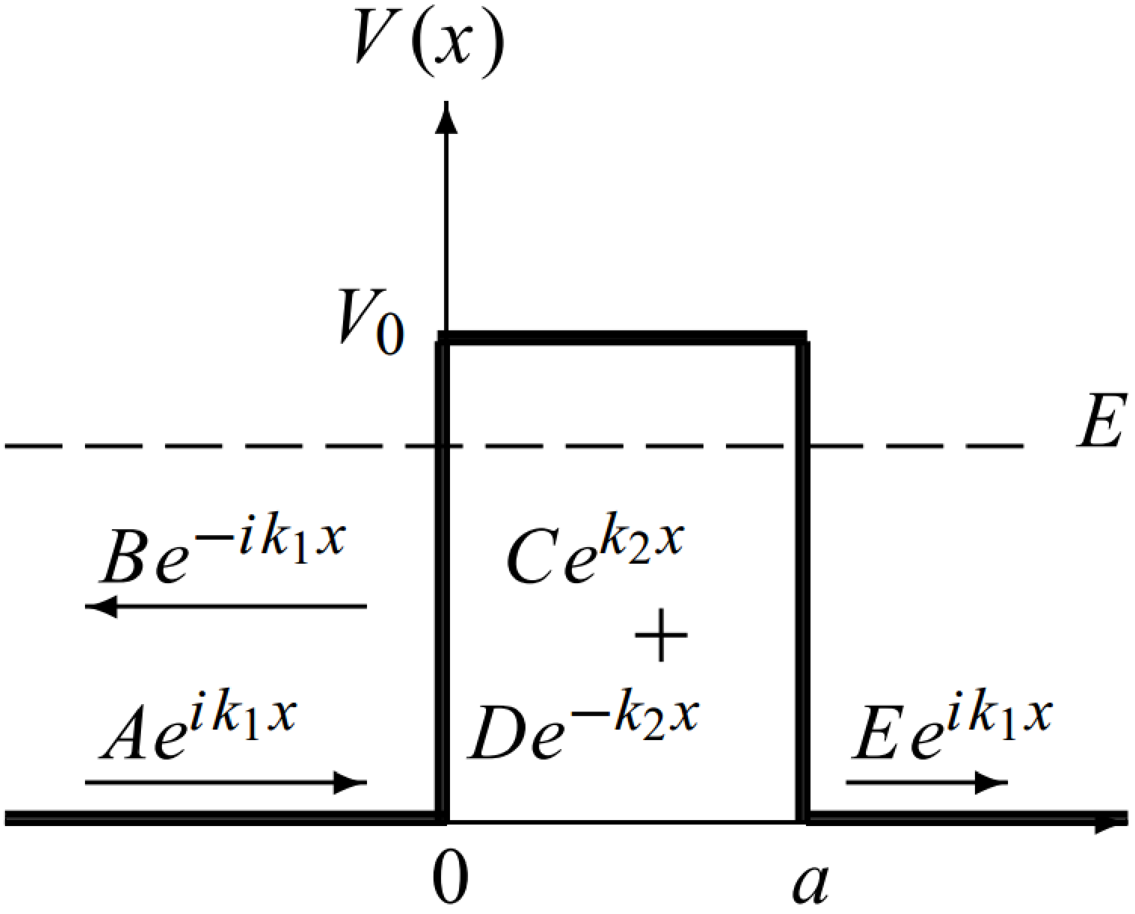
$$V(x) = \begin{cases} 0, & x < 0, \\ V_0, & 0 \le x \le a, \\ 0, & x > a. \end{cases}$$

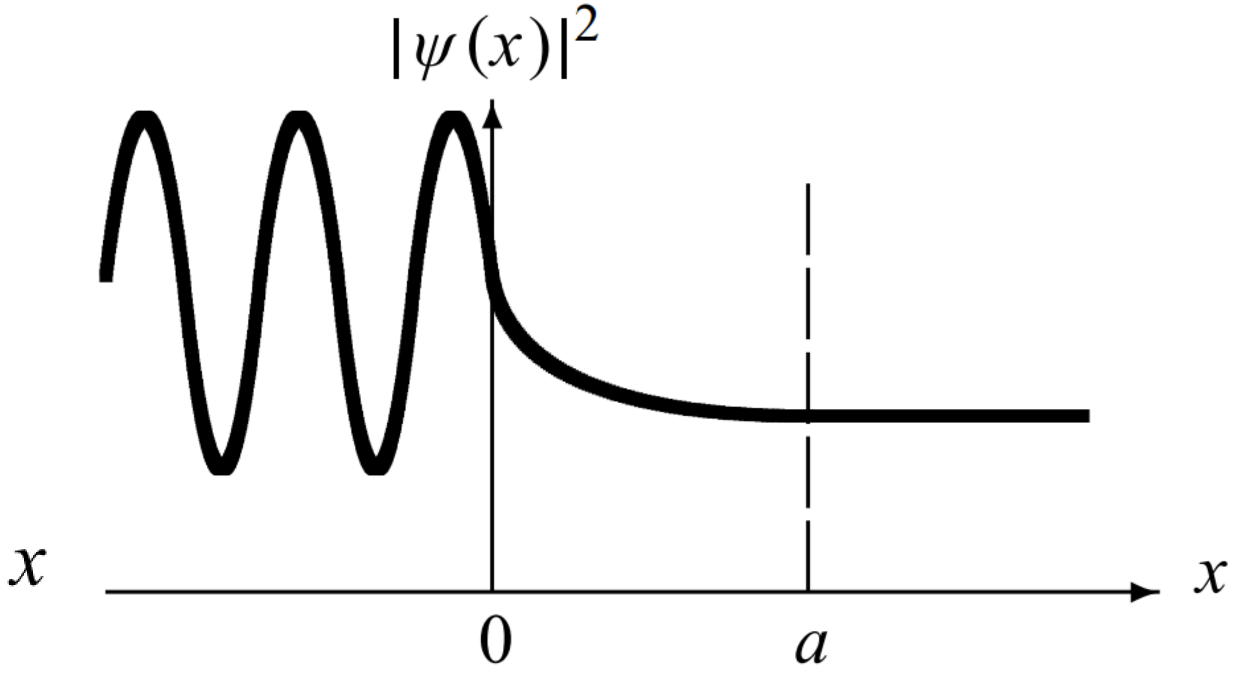
(a) Case $E > V_0$

(b) Case $E < V_0$



The potential barrier: (b) Case $E < V_0$





The potential barrier: (b) Case $E < V_0$

$$\psi(x) = \begin{cases} \psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}, & x \leq 0, \\ \psi_2(x) = Ce^{k_2x} + De^{-k_2x}, & 0 < x < a, \\ \psi_3(x) = Ee^{ik_1x}, & x \geq a, \end{cases}$$

where $k_1^2 = 2mE/\hbar^2$ and $k_2^2 = 2m(V_0 - E)/\hbar^2$.

The potential barrier: (b) Case $E < V_0$

The continuity conditions of the wavefunction and its derivative at $x = 0$ and $x = a$ yield

$$\begin{aligned} A + B &= C + D, \\ ik_1(A - B) &= k_2(C - D), \\ Ce^{k_2 a} + De^{-k_2 a} &= Ee^{ik_1 a}, \\ k_2\left(Ce^{k_2 a} - De^{-k_2 a}\right) &= ik_1 Ee^{ik_1 a}. \end{aligned}$$

The potential barrier: (b) Case $E < V_0$

With some calculations the coefficients R and T become

$$R = \left(\frac{k_1^2 + k_2^2}{k_1 k_2}\right)^2 \sinh^2(k_2 a) \left[4\cosh^2(k_2 a) + \left(\frac{k_2^2 - k_1^2}{k_1 k_2}\right)^2 \sinh^2(k_2 a)\right]^{-1}$$

$$T = \frac{|E|^2}{|A|^2} = 4\left[4\cosh^2(k_2 a) + \left(\frac{k_2^2 - k_1^2}{k_1 k_2}\right)^2 \sinh^2(k_2 a)\right]^{-1} .$$

The potential barrier: (b) Case $E < V_0$

We can rewrite R in terms of T as

$$R = \frac{1}{4} T \left(\frac{k_1^2 + k_2^2}{k_1 k_2} \right)^2 \sinh^2(k_2 a).$$

Since $\cosh^2(k_2 a) = 1 + \sinh^2(k_2 a)$ we can write

$$T = \left[1 + \frac{1}{4} \left(\frac{k_1^2 + k_2^2}{k_1 k_2} \right)^2 \sinh^2(k_2 a) \right]^{-1} .$$

The potential barrier: (b) Case $E < V_0$

$$\left(\frac{k_1^2 + k_2^2}{k_1 k_2}\right)^2 = \left(\frac{V_0}{\sqrt{E(V_0 - E)}}\right)^2 = \frac{V_0^2}{E(V_0 - E)}$$

$$\lambda = a\sqrt{2mV_0/\hbar^2} \text{ and } \varepsilon = E/V_0$$

The potential barrier: (b) Case $E < V_0$

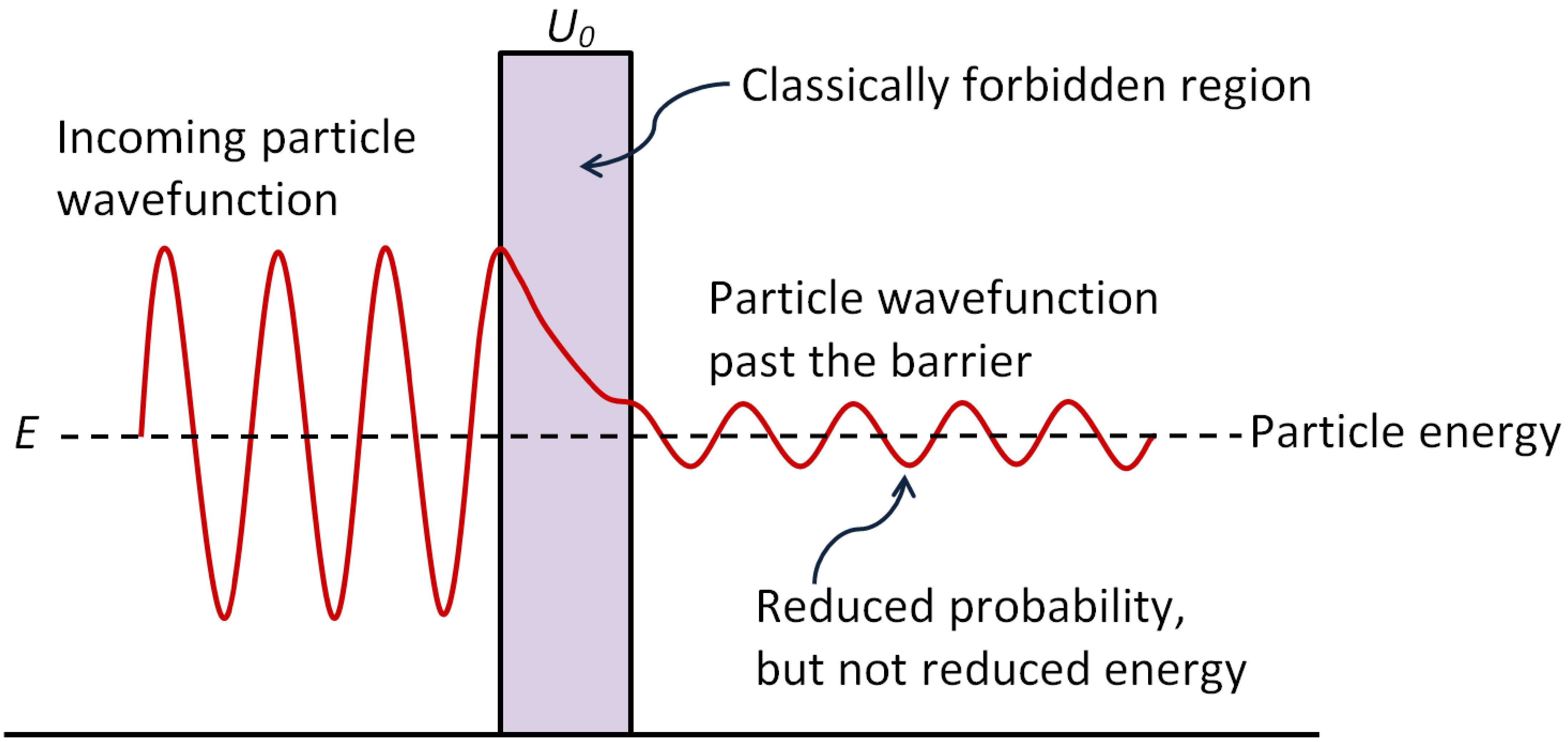
$$R = \frac{T}{4\varepsilon(1-\varepsilon)} \sinh^2\left(\lambda\sqrt{1-\varepsilon}\right),$$

$$T = \left[1 + \frac{1}{4\varepsilon(1-\varepsilon)} \sinh^2\left(\lambda\sqrt{1-\varepsilon}\right)\right]^{-1}$$

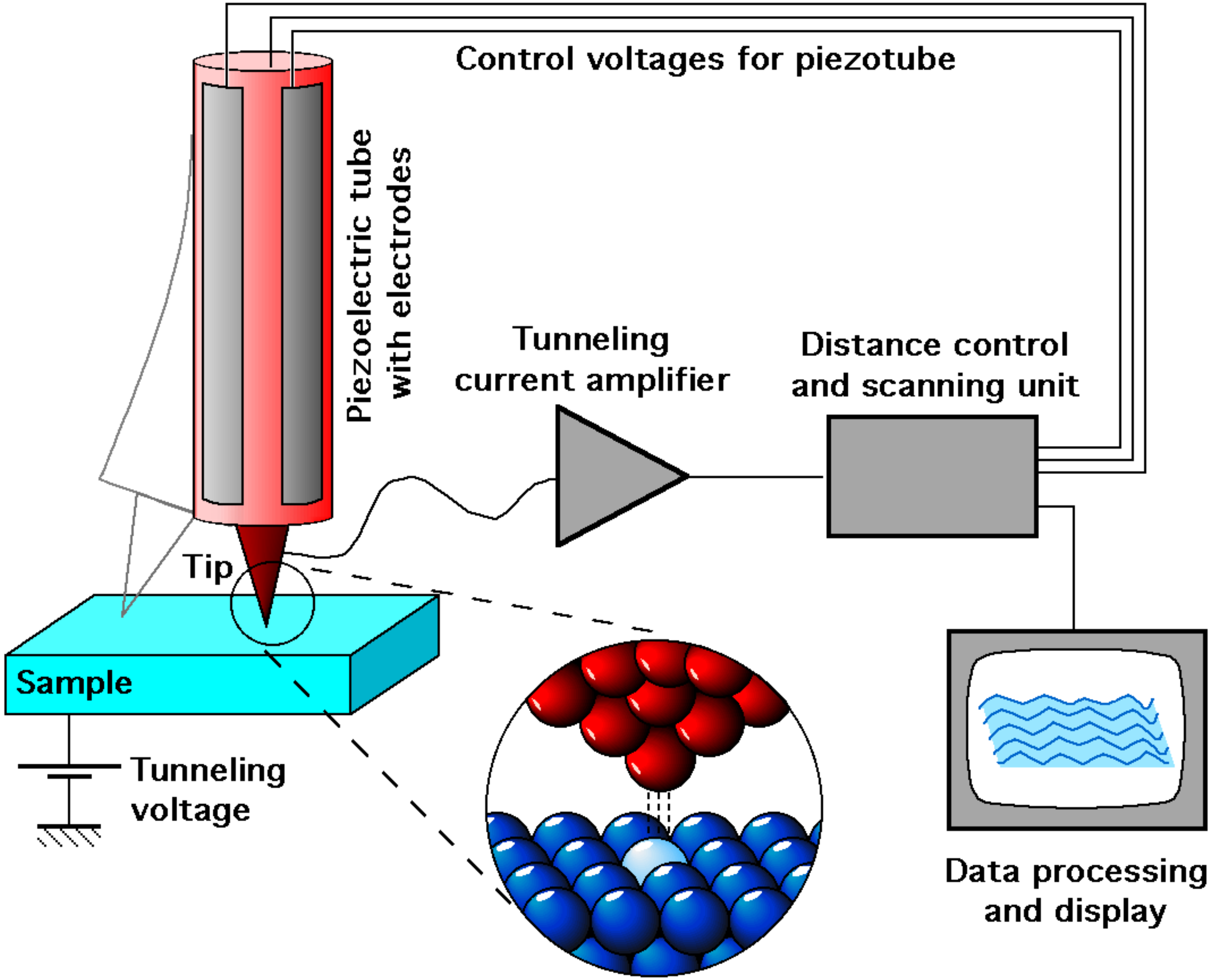
The Tunneling Effect

The tunneling effect consists of the propagation of a particle through a region where the particle’s energy is smaller than the potential energy. Classically this region is forbidden to the particle where its kinetic energy would be negative. Quantum mechanically, however, since particles display wave features, the quantum waves can tunnel through the barrier.

The Tunneling Effect



Scanning tunnelling microscopy (STM)



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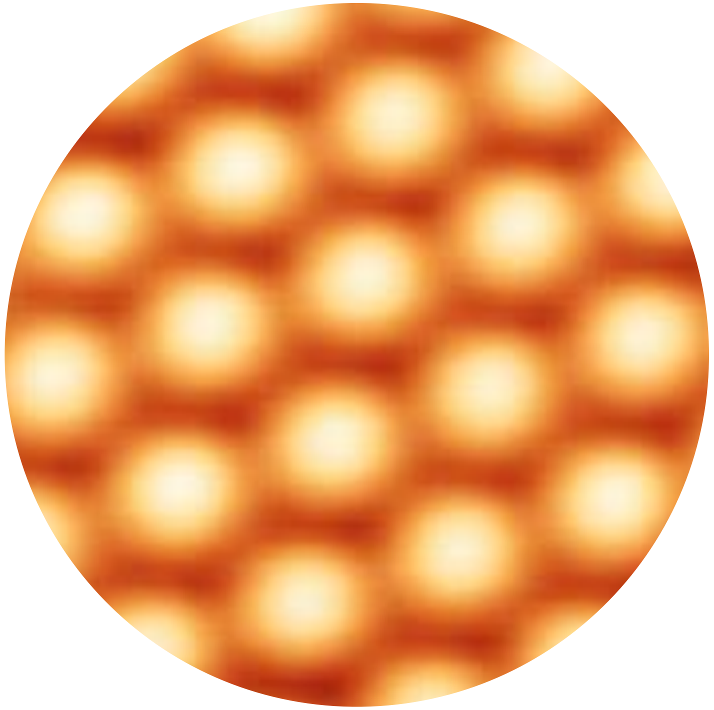
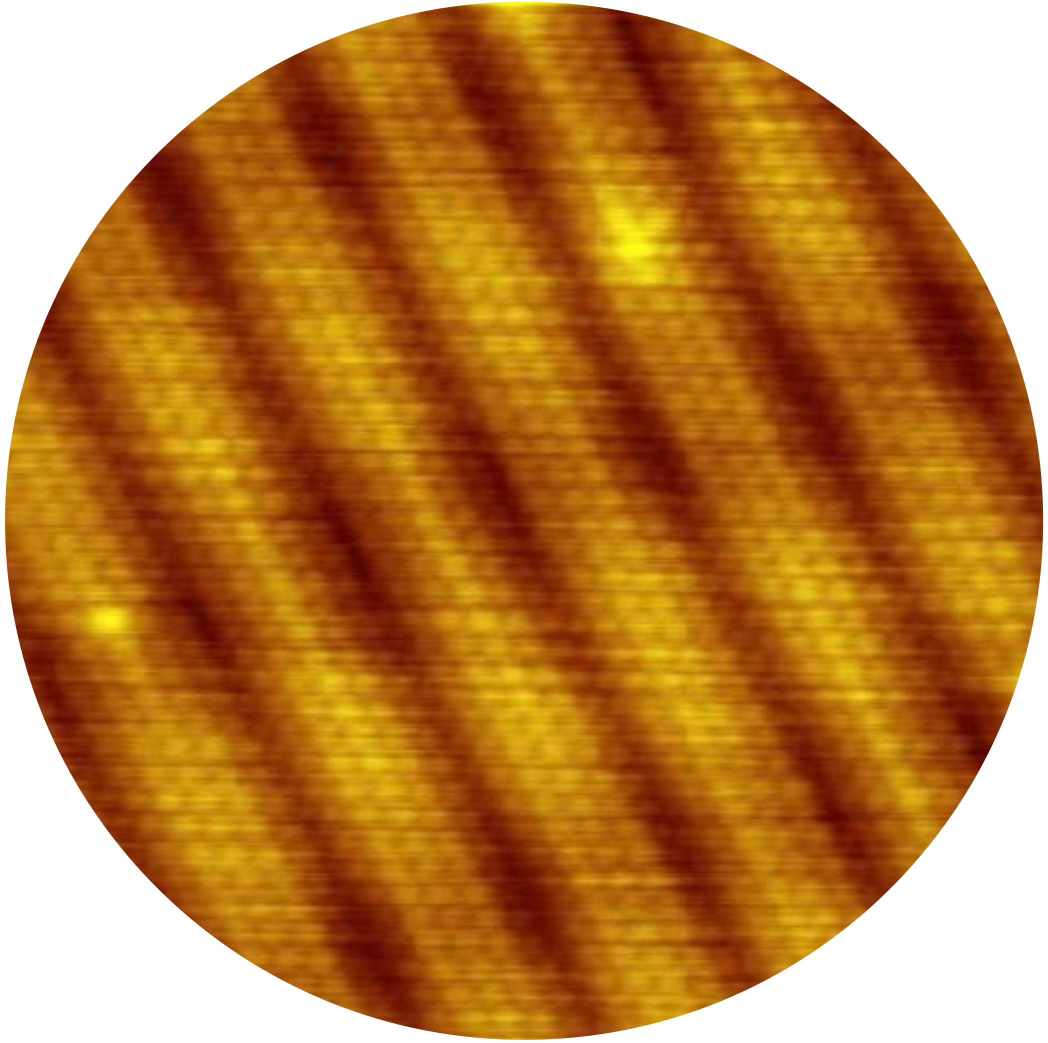
Si & Au as seen in STM





wikipedia.org

Problem 4.1

A particle moving in one dimension is in a stationary state whose wave function

$$\psi(x) = \begin{cases} 0, & x < -a, \\ A\left(1 + \cos \frac{\pi x}{a}\right), & -a \leq x \leq a, \\ 0, & x > a, \end{cases}$$

where A and a are real constants.

(a) Is this a physically acceptable wave function? Explain.
(b) Find the magnitude of A so that $\psi(x)$ is normalized.
(c) Evaluate Δx and Δp. Verify that $\Delta x \Delta p \geq \hbar/2$.
(d) Find the classically allowed region.

Problem 4.3

An electron is moving freely inside a one-dimensional infinite potential box with walls at $x = 0$ and $x = a$. If the electron is initially in the ground state ($n = 1$) of the box and if we *suddenly* quadruple the size of the box (i.e., the right-hand side wall is moved instantaneously from $x = a$ to $x = 4a$), calculate the probability of finding the electron in:

(a) the ground state of the new box and

(b) the first excited state of the new box.