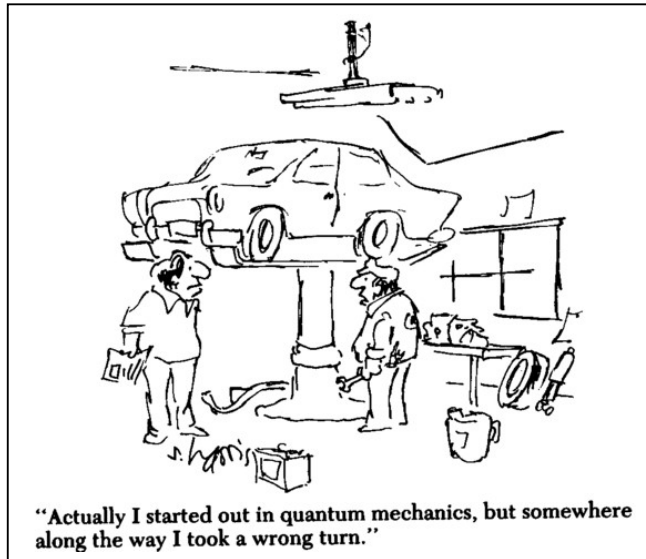


Introductory Quantum mechanics



Probabilistic interpretation of the matter waves

In wave picture the intensity of radiation I is proportional to $\overline{E^2}$, where $\overline{E^2}$ is the average value over one cycle of the square of the electric field strength of the EM wave, ($E = E_0 \sin(kx - \omega t) \Rightarrow \overline{E^2} = \frac{1}{T} \int_0^T E^2 dt$).

In photon picture, $I = Nh\nu$; N = average number of photons per unit time crossing unit area perpendicular to the direction of propagation.

Correspondence principle says that (what is explained in the wave picture has to be consistent with what is explained in the photon picture)

$$I = Nh\nu = \epsilon_0 c \overline{E^2}.$$


Since the probability of observing a photon at a point in a unit time is proportional to N , the probability of observing a photon is $\propto N \propto \overline{E^2}$, i.e. the probability of observing a photon at any point in space is proportional to the square of the averaged electric field strength at that point.

In exact analogy to the statistical interpretation of radiation as argued above, the square of the amplitude of

the matter wave of a particle, $|\Psi|^2$ (Ψ is called the *wave function*) is interpreted as the probability density of observing a material particle. If the wave function at the location x , the probability that the particle could be observed between x and $x + dx$ is given by $|\Psi(x)|^2 dx$.

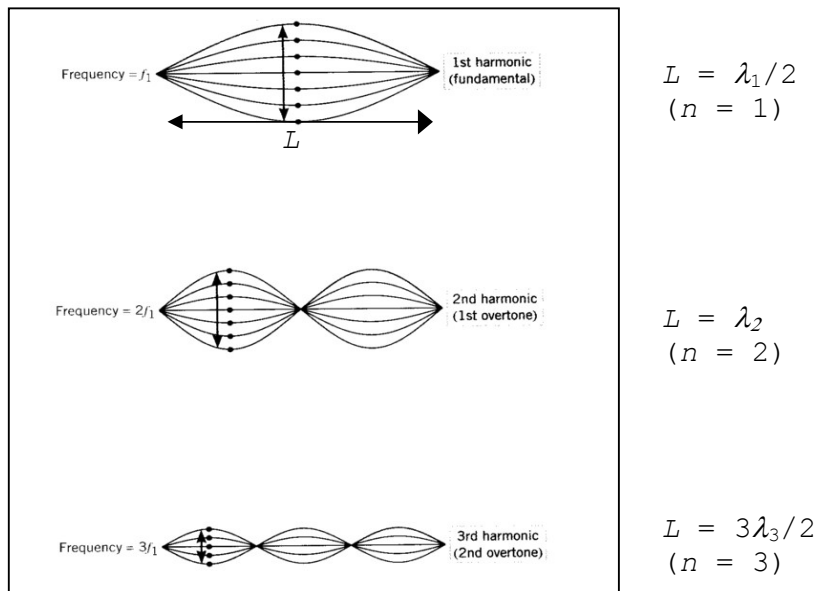
Probability for a particle to be found between x and $x + dx = |\Psi(x,t)|^2 dx$

Hence, a particle's wave function gives rise to a *probabilistic interpretation* of the position of a particle (due to Max Born in 1926).

	<p>German-British physicist who worked on the mathematical basis for quantum mechanics. Born's most important contribution was his suggestion that the absolute square of the wavefunction in the Schrödinger equation was a measure of the probability of finding the particle at a given location. Born shared the 1954 Nobel Prize in physics with Bothe</p>
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Quantum description of a particle in an infinite well

Description of standing waves which ends are fixed at $x = 0$ and $x = L$. (for standing wave, the speed is constant), $v = \lambda\nu = \text{constant}$)

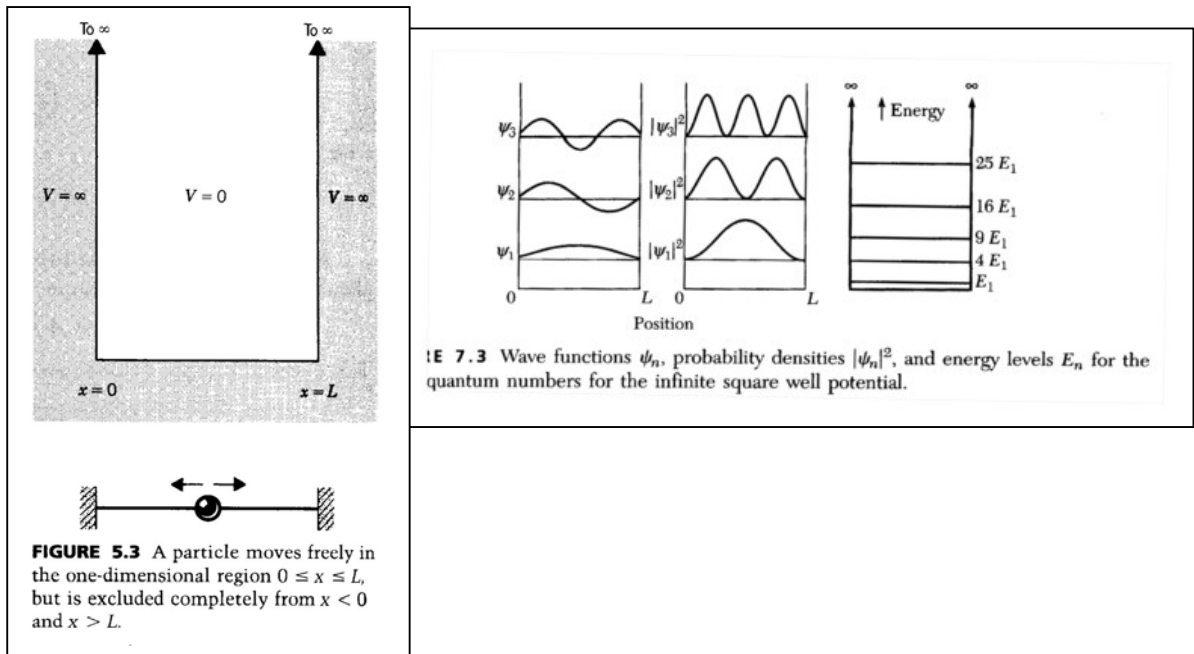


In general, the equation that describes a standing wave is simply:

$$L = n\lambda_n/2, \tag{SW}$$

where the length of the system L is fixed, λ_n is the wavelength associated with the n mode standing wave, $n = 1, 2, \dots$ is the 'quantum number' (so called because the number is 'quantised' - meaning that it takes only discrete value and is not a continuous variable. n characterises the mode of the standing wave (e.g. $n = 1$ is the fundamental mode, $n = 2$ is the second harmonics etc.)

Treat the particle as a wave described by its wave function, ψ . A particle confined in a 'quantum well' (infinitely hard wall with a width L) forms stationary (standing) wave in the well in the similar manner to the classical stationary wave:

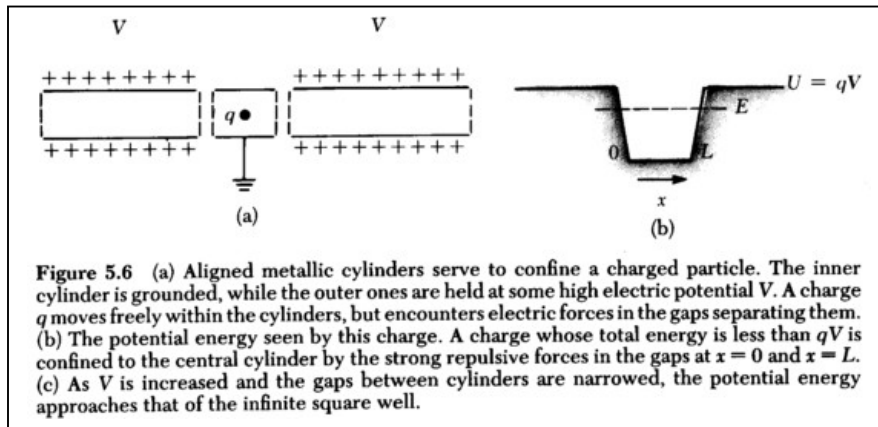


The particle in the well is confined to

$$0 < x < L$$

The infinitely hard walls correspond to an infinite potential energy $V \rightarrow \infty$ at $x = 0$ and $x = L$:

$$V(x) = \begin{cases} \infty, & x \leq 0, x \geq L \\ 0, & 0 < x < L \end{cases}$$



The confined particle is "free" between $0 < x < L$, i.e. the potential that acts on the particle in this range is 0 (or, in other words, the force acting on the particle is zero, according to $F = -\frac{\partial V}{\partial x}$).

In the box, the particle has all of its mechanical energy in the form of kinetic energy only. No exchange of mechanical energy ($K \leftrightarrow V$) is happening within the box (nor at the boundary) because $V = 0$ in the box. (Recall from classical mechanics that the total mechanical energy of a system = potential energy + kinetic energy.)

Mathematically, we write this as

$$E = K + V = p^2/2m + 0 = p^2/2m$$

(conservation of total mechanical energy)

Due to the probabilistic interpretation of the wave function, $P(x) = |\psi|^2$ is always > 0 except at the boundaries.

Probability to find the particle between x_1 and $x_2 =$

$$\int_{x_1}^{x_2} P(x) dx = \int_{x_1}^{x_2} |\psi(x)|^2 dx$$

e.g., For $n = 1$ quantum state, the probability to find the particle is highest at $x = L/2$.

For $n = 2$ quantum state, the probability to find the particle is highest at points $x = L/4$ and $x = 3L/4$, etc.

The particle which is bouncing back and forth between the walls must exist within somewhere within the well, hence

$$\int_{-\infty}^{\infty} P(x) dx = \int_0^L |\psi(x)|^2 dx = 1$$

⇒ Normalisation condition for the wave function

According to the probabilistic interpretation of the particle's existence along the x-axis, if we make many measurements repeatedly to determine the position of the particle in the box (each measurement is made on a new box with similar physical parameters), the probable outcome is predicted to be

$$\bar{x} = \int_{-\infty}^{\infty} x |\psi(x)|^2 dx$$

By analogy, the average value of any function of x can be found:

$$\overline{f(x)} = \int_{-\infty}^{\infty} f(x) |\psi(x)|^2 dx$$

Expectation value of $f(x)$

Due to the standing wave condition in Eq. (SW), the momentum of the particle is also quantised:

$$p_n = \frac{h}{\lambda_n} = \frac{nh}{2L}$$

It follows that the total energy of the particle is also quantised:

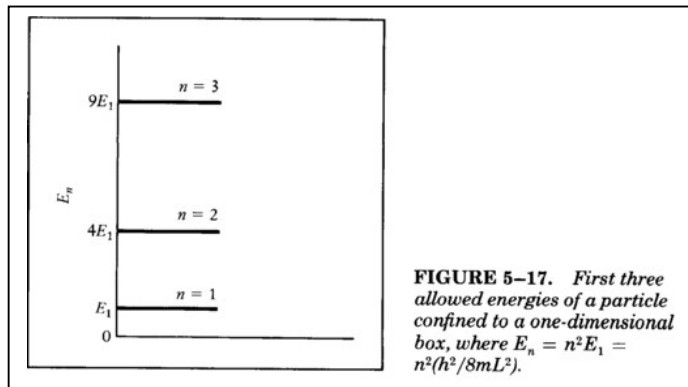
$$E_n = \frac{p_n^2}{2m} = n^2 \frac{\pi^2 \hbar^2}{2mL^2},$$

(where $\hbar = h/2\pi$). The $n = 1$ state is a characteristic state called the ground state = state with lowest possible energy. Ground state is always used as the reference state when we refer to "excited states" ($n = 2, 3$ or higher).

Hence the total energy of the n -th state, expressed in term of the ground state energy (also called zero-point

energy), $E_0 = \frac{\pi^2 \hbar^2}{2mL^2}$, is

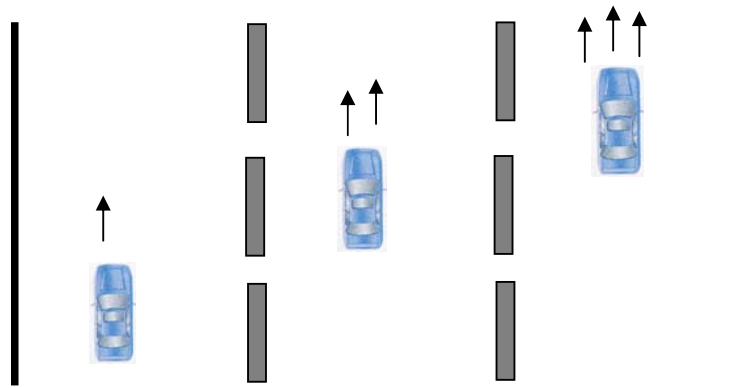
$$E_n = n^2 E_0 \quad (n = 1, 2, 3, 4, \dots)$$



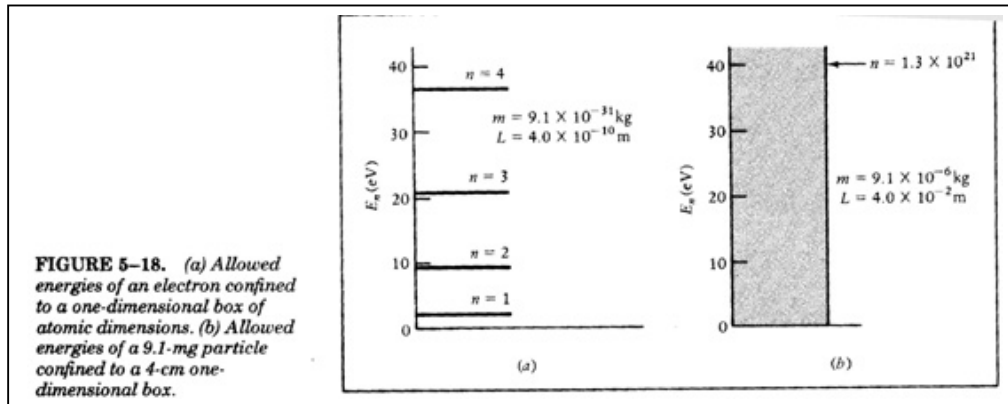
Note for notational purposes, $n = 1$ corresponds to the ground state, ($E_1 \equiv E_0$), $n = 2$ corresponds to the first excited state, etc.

Note that lowest possible energy for a particle in the box is not 0 but E_0 due to the Heisenberg uncertainty principle (see the lecture note when we discussed the Heisenberg uncertainty)

ANALOGY: Cars moving in the right lane on the highway are in 'excited states' as they must travel faster (at least according to the traffic rules). Cars travelling in the left lane are in the 'ground state' as they can move with a relaxingly lower speed. Cars in the excited states must finally resume to the ground state (i.e. back to the left lane) when they slow down.



Since the energy level is very small (e.g. for an electron trapped within the size of a typical atom, 4 \AA , $E_0 \sim 4 \times 10^{-8} \text{ eV}$). The spacing between adjacent energy levels is so tiny that their quantisation is too fine to be discerned from macroscopic point of view - the energy levels just appear continuous.



The problem of the particle in the box is an artificial physical system but nevertheless it reveals the fundamental feature that a quantum system that is bounded between some boundaries would have their energy levels quantised.



Schrödinger, Erwin (1887-1961), Austrian physicist and Nobel laureate. Schrödinger formulated the theory of wave mechanics, which describes the behavior of the tiny particles that make up matter in terms of waves. Schrödinger formulated the Schrödinger wave equation to describe the behavior of electrons (tiny, negatively charged particles) in atoms. For this achievement, he was awarded the 1933 Nobel Prize in physics with British physicist [Paul Dirac](#)

The Schrodinger Equation

Now we generalise the above description to a general case in which a particle is subjected to some potential within some boundaries which are in general not infinite. We wish to derive a mathematical formulation to describe the wave function of a particle system, hence allowing us to gain fundamental insight into their behaviour which could be verified against experimental observation (e.g. its quantised energies, momentum etc.)

The mathematical description that governs the behaviour of a wave function within a system has to satisfy some criteria:

- 1) Energy must be conserved: $E = K + U$
- 2) Must be consistent with de Broglie hypothesis that $p = h/\lambda$
- 3) Mathematically well-behaved and sensible (e.g. finite, single valued, linear so that superposition prevails, conserved in probability etc.)

We shall derive the equation that describes the wave function (conforming to the above criterion) by taking direct analogy of a wave $\Psi(x,t)$ propagating in the x -direction:

$$\frac{\partial^2 \Psi}{\partial x^2} = \frac{1}{c^2} \frac{\partial^2 \Psi}{\partial t^2}$$

(FWV)

Eq.(FWV) is the well-known 1-D differential wave equation, where c is the velocity of the propagating wave, $c = \omega/k$. [A special case for the solution to Eq.(FEV) is the plain wave solution which we are familiar with, $\Psi(x,t) = A \cos(kx - \omega t - \phi)$. However, in general, the solution of the wave function is not necessarily a plain wave; it could takes on form which is otherwise, depending on the boundary conditions of the system]

We will take the form of Eq.(FWN) as the basis to derive the equation that governs the wave function of a particle with a conserved energy E and which is bound by some potential within some region of space.

Conserved E means that the frequency of the wave function is sharp (precisely defined) and constant: $\nu = E/h$.

As a standard practice in solving second order differential equation, we use the method of separation of variables by separating the solution into a purely spatial part and a purely time-dependent part:

$$\Psi(x,t) = \psi(x)\phi(t)$$

$\phi(t)$ describes the time-dependent part of the wave function, and is given by $\phi(t) = \cos \omega t$ where $\omega = 2\pi\nu$.

Plug $\Psi(x,t)=\psi(x)\phi(t)$ into Eq.(FWV) and go through some mathematics,

$$\frac{\partial^2\psi(x)}{\partial x^2} = -\left(\frac{p}{\hbar}\right)^2 \psi(x) \tag{SE1}$$

The particle is interacting with the point-dependent potential $V(x)$, hence the total energy is

$$E = V + K = V + p^2/2m$$

$$\Rightarrow p^2 = 2m(E-V)$$

Substitute for Eq.(SE1), we have

$$\frac{\hbar^2}{2m} \frac{\partial^2\psi(x)}{\partial x^2} + (E-V)\psi(x) = 0 \tag{SE}$$

1-D, non-relativistic, time-independent Schrodinger equation

Eq.(SE) is the differential equation we are looking for that govern the quantum behaviour of a microscopic particle subjected to x-dependent potential $V(x)$.

Note that for a particle subjected to a potential $V(x)$, the wavelength associated with the wave function is modified to

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2m(E-V)}}$$

Armed with Eq.(SE), we now revisit the particle in the infinite well. By using appropriate boundary condition to Eq.(SE), the solution should reproduce the quantisation of energy level as have been deduced earlier.

The infinite quantum well correspond to $V(x)=0$ in Eq.(SE)

$$\frac{d^2\psi(x)}{dx^2} = -B^2\psi(x), \text{ where } B^2 = \frac{2mE}{\hbar^2} \tag{QWSE}$$

From the studies of second order differential equation, the general solution to Eq. (QWSE) is

$$\psi(x) = A \sin Bx + C \cos Bx$$

where A, C are two arbitrary constant that is to be determined by the boundary condition that $\psi(x=0)=\psi(x=L)=0$.

From $\psi(x=0)=0, C=0$;

To fulfil $\psi(x=L)=0, BL = n\pi$ where $n = 1, 2, 3, \dots$

$$\Rightarrow E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2} \quad (\text{En})$$

This is just the quantisation of energy levels as we have seen earlier, which we now re-derived more formally by solving the S.E.

QUESTION: the energy of the system, according to Eq. (En), is dependent on the current energy state (ie. the value of n). Is energy being conserved here?

The solution of the wave function is $\psi_n(x) = A_n \sin \frac{n\pi x}{L}$.

(Prove this yourself. Can we take $\psi_n(x) = B_n \cos n \frac{n\pi x}{L}$ as the solution? Why?) The constant A_n can be found by the normalisation condition.

$$\psi_n(x) = A_n \sin \frac{n\pi x}{L}$$

$$\int_{-\infty}^{\infty} \psi_n^2(x) dx = \int_0^L \psi_n^2(x) dx = A_n^2 \int_0^L \sin^2 \left(\frac{n\pi x}{L} \right) dx = \frac{A_n^2 L}{2} = 1$$

$$A_n = \sqrt{\frac{2}{L}}$$

ANSWER THIS QUESTION: How would you describe, using SE, a free particle that is not bounded by any potential? What is the wave function of such a free particle?

Example

An electron is trapped in a one-dimensional region of length 1.0×10^{-10} m. (a) How much energy must be supplied to excite the electron from the ground state to the first state? (b) In the ground state, what is the probability of finding the electron in the region from $x = 0.090 \times 10^{-10}$ m to 0.110×10^{-10} m? (c) In the first excited state, what is the probability of finding the electron between $x = 0$ and $x = 0.250 \times 10^{-10}$ m? (d) Show that the average value of x is $L/2$, independent of the quantum state.

ANS

(a) $E_0 = \frac{\hbar^2 \pi^2}{2mL^2} = 37 \text{ eV}; \quad E_2 = n^2 E_0 = (2)^2 E_0 = 148 \text{ eV}$

$\Rightarrow \Delta E = E_2 - E_0 = 111 \text{ eV}$

(NOTE: the subscript "0" and "1" denotes the same state - the ground state)

(b) $\int_{x_1}^{x_2} \psi_0^2 dx = \frac{2}{L} \int_{x_1}^{x_2} \sin^2 \frac{\pi x}{L} dx = \left(\frac{x}{L} - \frac{1}{2\pi} \sin \frac{2\pi x}{L} \right) \Big|_{x_1}^{x_2} = 0.0038$

(c) $\psi_2 = \frac{2}{L} \sin^2 \frac{2\pi x}{L};$

$\int_{x_1}^{x_2} \psi_2^2 dx = \frac{2}{L} \int_{x_1}^{x_2} \sin^2 \frac{2\pi x}{L} dx = \left(\frac{x}{L} - \frac{1}{4\pi} \sin \frac{4\pi x}{L} \right) \Big|_{x_1}^{x_2} = 0.25$

(d) $\bar{x} = \int_0^L x |\psi_n|^2 dx = \frac{2}{L} \int_0^L x \sin^2 \frac{n\pi x}{L} dx = \frac{L}{2}$ (integration by parts)

(Hence a measurement of the average position of the particle yields no information about its quantum state.)

Particle in a 1-D finite potential well

In real physical system the potential energy seen by a trapped electron is not infinite

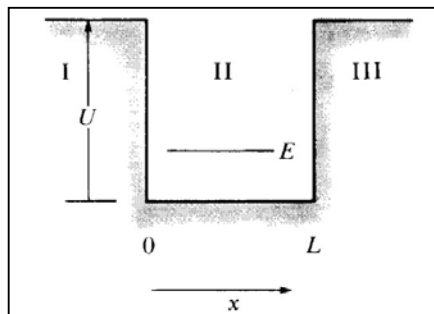


Figure 5.10 Potential energy diagram for a well of finite height U and width L . The energy E of the particle is less than U .

This is like putting a bouncing ball with total energy E (which is comprised purely of kinetic energy K) inside a box of high $|V|$. Classically, for the particle to remain trapped inside the finite square well ("bounded by the potential"), the necessary requirement is $E = K < |V|$. In

other words, if the total energy of the ball $E > |V|$, the ball would have gained enough energy to escape from the well (no more bounded). Also, since energy is conserved, the total energy $E = K + V = \text{constant}$.

Classically, as long as $E < |V|$, the particle is nowhere to be found outside the region $L < 0, x > L$. (common sense, right?)

Mathematically, the finite potential well takes on the form

$$V(x) = \begin{cases} 0, & x \leq 0, x \geq L \\ U, & 0 < x < L \end{cases}$$

Inside the well (region II),

$$\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + E\psi(x) = 0$$

Outside the well (region I, III),

$$\frac{\partial^2 \psi(x)}{\partial x^2} = \frac{2m}{\hbar^2} (U - E)\psi(x) = C^2 \psi(x),$$

where the constant at the RHS is positive. Solution to SE in region I, III is (recall, again, your differential equation) has the general form

$$\psi(x) = K_1 \exp(Cx) + K_2 \exp(-Cx)$$

Putting in boundary condition that the wave function has to be finite

- (A) as $x \rightarrow \infty$ in region III, and
- (B) as $x \rightarrow -\infty$ in region I

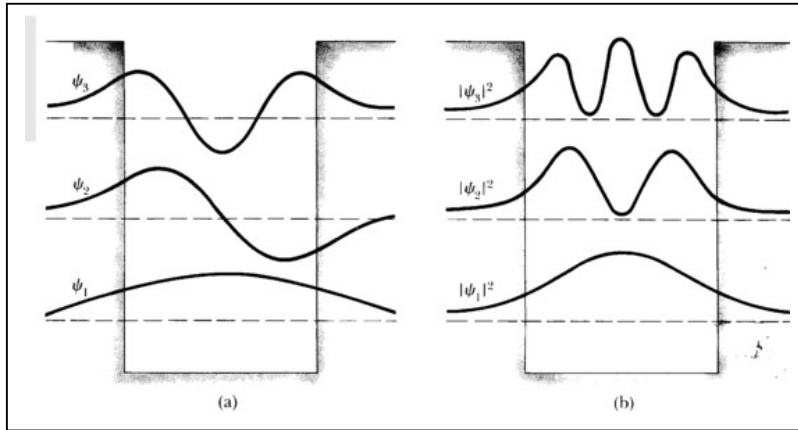
we arrive at
$$\psi(x) = \begin{cases} A_+ \exp(Cx), & x \leq 0 \\ A_- \exp(-Cx), & x \geq L \end{cases}$$

NOTE: $\psi(x)$ is NON-ZERO outside the classically "forbidden" region, but an exponentially decaying function. There is some finite probability to find the particle outside the box - something not possible in classical mechanics. This is the famous QUANTUM TUNNELLING EFFECT.

The complete wave function for the well is sinusoidal in the well and decaying exponentially outside. The inside and outside wave functions have to be joined smoothly at the walls:

$$\psi_{\text{inside}} = \psi_{\text{outside}}, \quad \left. \frac{d\psi}{dx} \right|_{\text{inside}} = \left. \frac{d\psi}{dx} \right|_{\text{outside}}$$

(boundary conditions at the boundaries)



The corresponding allowed energy states are somewhat lower than that of the infinite well because of a greater wavelength inside the box (explain why this is so)

The number of bounded energy states is finite. Bound states can exist only for $E_n < U$ (in the infinite quantum well case, the number of bound state is infinite because U is infinitely large). Once the excited energy is larger than U , the particle is no more bounded but escaping from the box as a *free particle* (and is not described by a stationary wave anymore).

The weird tunnelling effect allows a confined particle within a finite potential well to penetrate through the classically impenetrable potential wall. This tunnelling probability is vanishingly small except at atomic scale, in particular of the width of the well is thin enough.

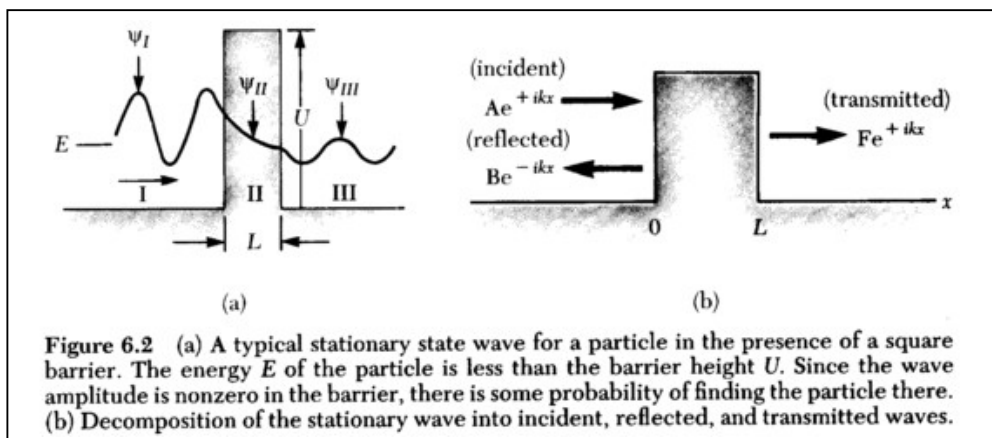
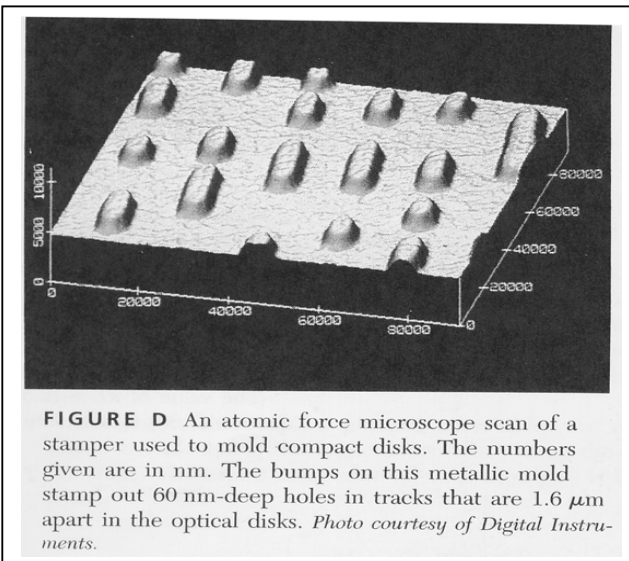
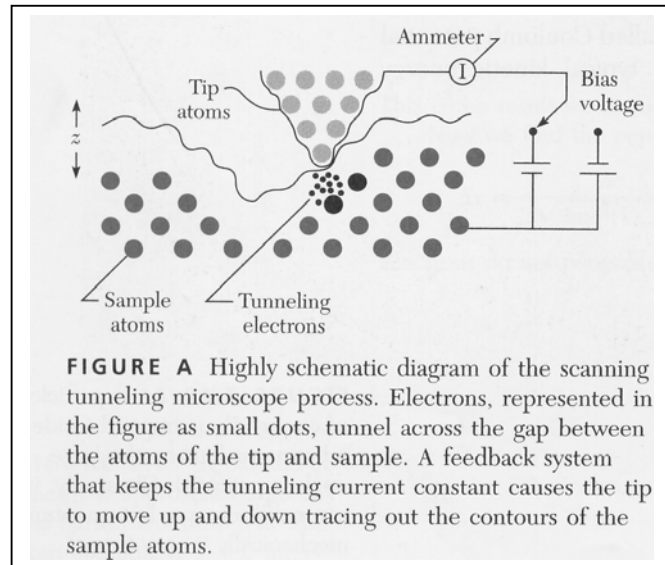
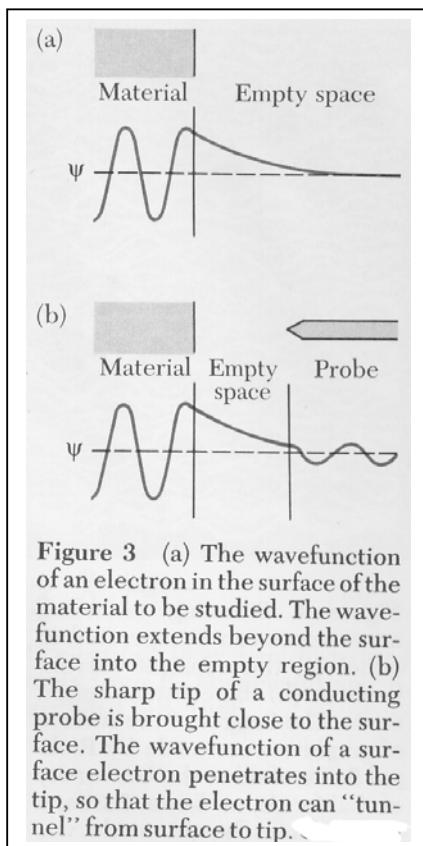
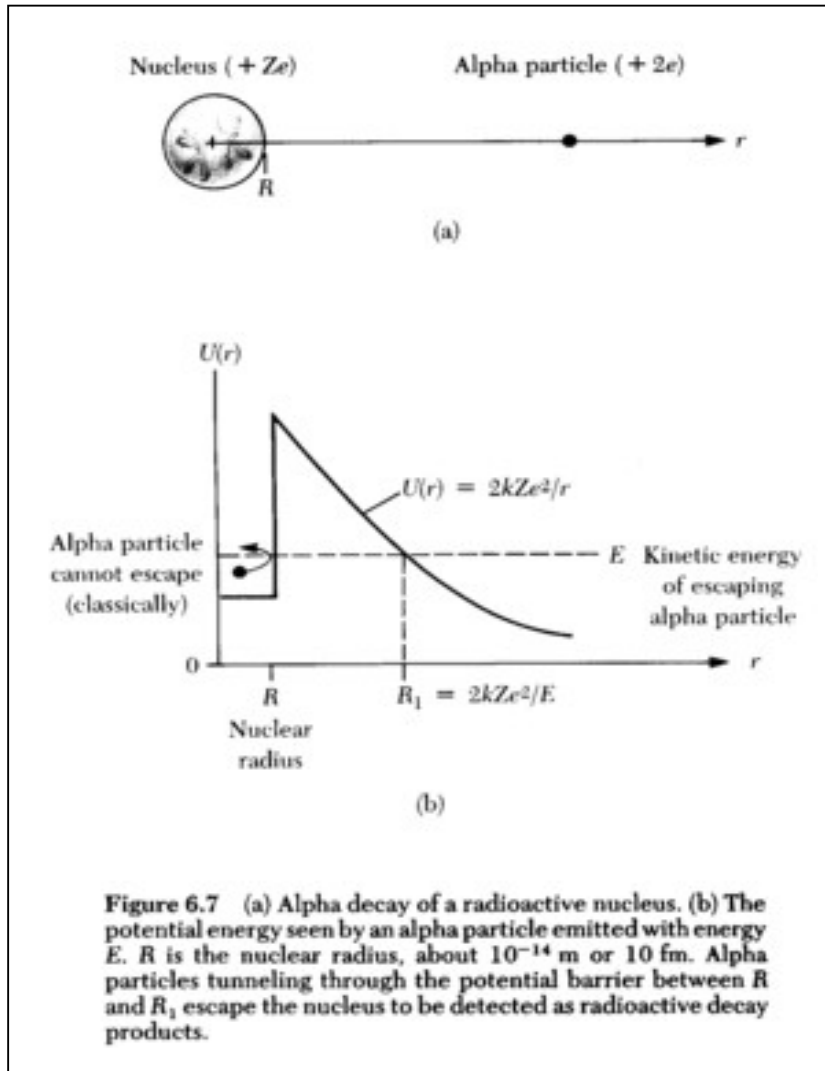


Figure 6.2 (a) A typical stationary state wave for a particle in the presence of a square barrier. The energy E of the particle is less than the barrier height U . Since the wave amplitude is nonzero in the barrier, there is some probability of finding the particle there. (b) Decomposition of the stationary wave into incident, reflected, and transmitted waves.

Quantum tunnelling effect has been utilised in Esaki tunnelling diode that can perform extremely fast calculation. It also explains the alpha decay of radioactive nucleus. It is the basis for STM (scanning tunnelling microscope)





As a generalisation to a highly simplified form of potential (infinite, finite square well), in fact we can appropriately model a atomic or nucleus system by treating the trapped particle by some effective potential (such as electrons bounded by the atomic potential and nucleons bounded inside a nucleus by the ``Yukawa potential``). We show below some examples of potential found in real physical system that bound system of particles together in *bound states*.

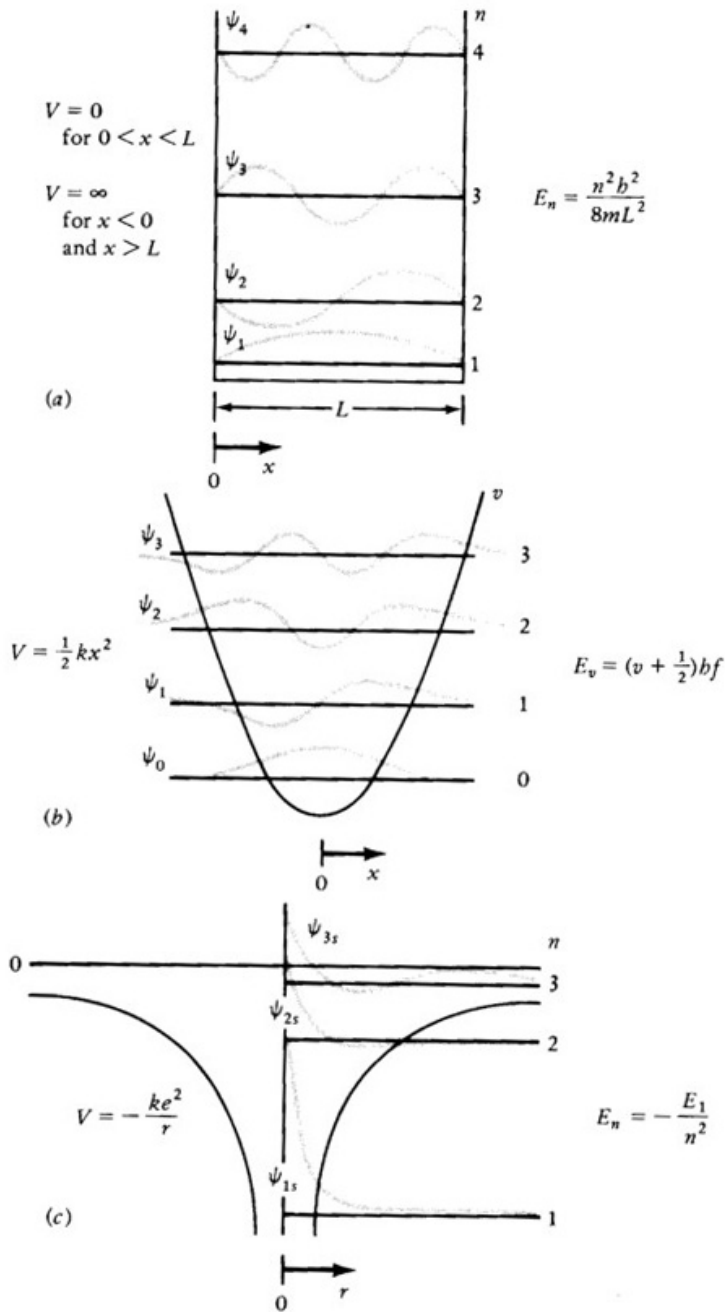
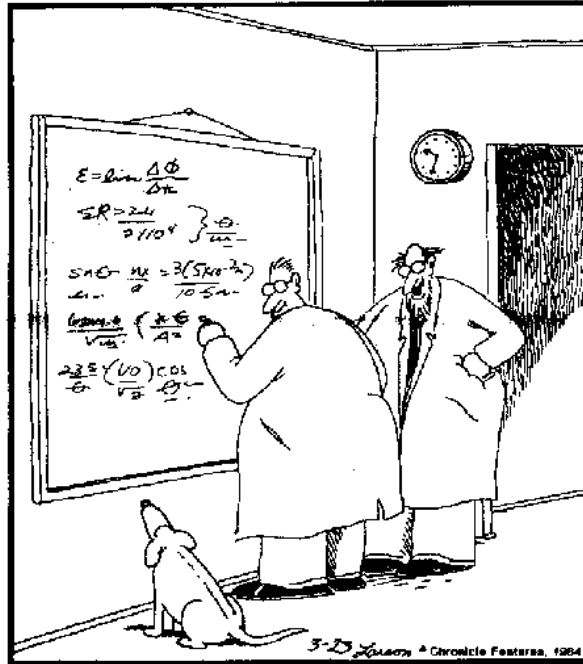


FIGURE 5-23. Potential-energy functions, wave functions, and allowed energies of three simple potential energies: (a) an infinitely deep well, (b) a simple harmonic oscillator, and (c) a particle subject to an inverse-square attractive force (hydrogen atom).

THE FAR SIDE

By GARY LARSON



"Ohhhhhhh . . . Look at that, Schuster . . .
Dogs are so cute when they try to comprehend
quantum mechanics."

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