$$\rho = |\psi|^2 \; ; \tag{2.32}$$

this choice implies:

$$\dot{\rho} = \psi^* \dot{\psi} + \psi \dot{\psi}^* \, .$$

If we assume, for instance, the wave equation corresponding to (2.29):

$$\dot{\psi} = \alpha\psi + \beta\nabla^2\psi \, , \tag{2.33}$$

we obtain:

$$\dot{\rho} = \psi^* \left(\alpha\psi + \beta\nabla^2\psi\right) + \psi \left(\alpha^*\psi^* + \beta^*\nabla^2\psi^*\right) \; .$$

If we also assume that the current probability density be

$$\boldsymbol{J} = \mathrm{i}k \left(\psi^* \boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^*\right) \; , \tag{2.34}$$

with k real so as to make $\boldsymbol{J}$ real as well, we easily derive

$$\boldsymbol{\nabla} \cdot \boldsymbol{J} = \mathrm{i}k \left(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*\right) \; .$$

It can be easily verified that the continuity equation (2.27) is satisfied if

$$\alpha + \alpha^* = 0 \, , \qquad \beta = -\mathrm{i}k \, . \tag{2.35}$$

It is of great physical interest to consider the case in which the wave function has more than two real components. In particular, the wave function of electrons has four components or, equivalently, two complex components. In general, the multiplicity of the complex components is linked to the existence of an intrinsic angular momentum, which is called *spin*. The various complex components are associated with the different possible spin orientations. In the case of particles with non-vanishing mass, the number of components is $2S+1$, where S is the spin of the particle. In the case of the electron, $S = 1/2$.

For several particles, as for the electron, spin is associated with a magnetic moment which is inherent to the particle: it behaves as a microscopic magnet with various possible orientations, corresponding to those of the spin, which can be selected by placing the particle in a non-uniform magnetic field and measuring the force acting on the particle.

2.4 Schrödinger's Equation

The simplest case to which our considerations can be applied is that of a non-relativistic free particle of mass m. To simplify notations and computations, we will confine ourselves to a one-dimensional motion, parallel for instance, to the x axis; if the particle is not free, forces will be parallel to the same axis as well. The obtained results will be extensible to three dimensions by exploiting the vector formalism. In practice, we will sistematically replace $\boldsymbol{\nabla}$ by its component $\nabla_x = \partial/\partial x \equiv \partial_x$ and the Laplacian operator $\nabla^2 =$

$\partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2$ by $\partial^2/\partial x^2 \equiv \partial_x^2$; the probability current density $\boldsymbol{J}$ will be replaced by J_x (J) as well. The inverse replacement will suffice to get back to three dimensions.

The energy of a non-relativistic free particle is

$$E = c\sqrt{m^2c^2 + p^2} \simeq mc^2 + \frac{p^2}{2m} + O\left(\frac{p^4}{m^3c^2}\right) ,$$

where we have explicitely declared our intention to neglect terms of the order of $p^4/(m^3c^2)$. Assuming de Broglie's interpretation, we write the wave function:

$$\psi_P(x,t) \sim \mathrm{e}^{2\pi\mathrm{i}(x/\lambda - \nu t)} = \mathrm{e}^{\mathrm{i}(px - Et)/\hbar} \tag{2.36}$$

(we are considering a motion in the positive x direction). Our choice implies the following wave equation

$$\dot{\psi}_P = -\frac{\mathrm{i}E}{\hbar}\psi_P = -\frac{\mathrm{i}}{\hbar}\left(mc^2 + \frac{1}{2m}p^2\right)\psi_P \,. \tag{2.37}$$

We have also

$$\partial_x \psi_P = \frac{\mathrm{i}}{\hbar} p \psi_P \,, \tag{2.38}$$

from which we deduce

$$\mathrm{i}\hbar\dot{\psi}_P = mc^2\psi_P - \frac{\hbar^2}{2m}\partial_x^2\psi_P \,. \tag{2.39}$$

Our construction can be simplified by multiplying the initial wave function by the phase factor $\mathrm{e}^{\mathrm{i}mc^2t/\hbar}$, i.e. defining

$$\psi \equiv \mathrm{e}^{\mathrm{i}mc^2t/\hbar}\psi_P \sim \exp\left(\frac{\mathrm{i}}{\hbar}\left(px - \frac{p^2}{2m}t\right)\right) \,. \tag{2.40}$$

Since the dependence on x is unchanged, ψ still satisfies (2.38) and has the same probabilistic interpretation as ψ_P. Indeed both ρ and J are unchanged. The wave equation instead changes:

$$\mathrm{i}\hbar\dot{\psi} = -\frac{\hbar^2}{2m}\partial_x^2\psi \equiv T\psi \,. \tag{2.41}$$

This is the *Schrödinger equation* for a free (non-relativistic) particle, in which the right-hand side has a natural interpretation in terms of the particle energy, which in the free case is only of kinetic type.

In the case of particles under the influence of a force field corresponding to a potential energy $V(x)$, the equation can be generalized by adding $V(x)$ to the kinetic energy :

$$\mathrm{i}\hbar\dot{\psi} = -\frac{\hbar^2}{2m}\partial_x^2\psi + V(x)\psi \,. \tag{2.42}$$

This is the one-dimensional Schrödinger equation that we shall apply to various cases of physical interest.

Equations (2.34) and (2.35) show that the probability density current does not depend on V and is given by:

$$J = -\frac{\mathrm{i}\hbar}{2m} \left(\psi^* \partial_x \psi - \psi \partial_x \psi^* \right) . \tag{2.43}$$

Going back to the free case and considering the *plane* wave function given in (2.36), it is interesting to notice that the corresponding probability density, $\rho = |\psi|^2$, is a constant function. This result is paradoxical since, by reducing (2.25) to one dimension, we obtain

$$\int_{-\infty}^{\infty} dx\ \rho(x,t) = \int_{-\infty}^{\infty} dx\ |\psi(x,t)|^2 = 1\ , \tag{2.44}$$

which cannot be satisfied in the examined case since the integral of a constant function is divergent. We must conclude that our interpretation excludes the possibility that a particle have a well defined momentum.

We are left with the hope that this difficulty may be overcome by admitting some (small) uncertainty on the knowledge of momentum. This possibility can be easily analyzed thanks to the linearity of Schrödinger equation. Indeed equation (2.41) admits other different solutions besides the simple plane wave, in particular the *wave packet* solution, which is constructed as a linear superposition of many plane waves according to the following integral:

$$\int_{-\infty}^{\infty} dp\ \tilde{\psi}(p) \exp\left(\frac{\mathrm{i}}{\hbar} \left(px - \frac{p^2}{2m} t \right) \right) .$$

The squared modulus of the superposition coefficients, $|\tilde{\psi}(p)|^2$, can be naturally interpreted, apart from a normalization constant, as the probability density in terms of momentum, exactly in the same way as $\rho(x)$ is interpreted as a probability density in terms of position.

Let us choose in particular a Gaussian distribution:

$$\tilde{\psi}(p) \sim \mathrm{e}^{-(p-p_0)^2/(4\Delta^2)}\ , \tag{2.45}$$

corresponding to

$$\psi_\Delta(x,t) = k \int_{-\infty}^{\infty} dp\ \mathrm{e}^{-(p-p_0)^2/(4\Delta^2)}\ \mathrm{e}^{\mathrm{i}\left(px - p^2 t/2m\right)/\hbar} . \tag{2.46}$$

where k must be determined in such a way that $\int_{-\infty}^{\infty} dx |\psi_\Delta(x,t)|^2 = 1$.

The integral in (2.46) can be computed by recalling that, if α is a complex number with positive real part ($Re\ (\alpha) > 0$), then

$$\int_{-\infty}^{\infty} dp\ \mathrm{e}^{-\alpha p^2} = \sqrt{\frac{\pi}{\alpha}}$$

and that the Riemann integral measure dp is left invariant by translations in the complex plane,

$$\int_{-\infty}^{\infty} dp\ \mathrm{e}^{-\alpha p^2} \equiv \int_{-\infty}^{\infty} d(p+\gamma)\ \mathrm{e}^{-\alpha(p+\gamma)^2}$$
$$= \int_{-\infty}^{\infty} dp\ \mathrm{e}^{-\alpha(p+\gamma)^2} = \mathrm{e}^{-\alpha\gamma^2} \int_{-\infty}^{\infty} dp\ \mathrm{e}^{-\alpha p^2} \mathrm{e}^{-2\alpha\gamma p}\,,$$

for every complex number γ. Therefore we have

$$\int_{-\infty}^{\infty} dp\ \mathrm{e}^{-\alpha p^2} \mathrm{e}^{\beta p} = \sqrt{\frac{\pi}{\alpha}} \mathrm{e}^{\beta^2/4\alpha}\,. \tag{2.47}$$

Developing (2.46) with the help of (2.47) we can write

$$\psi_\Delta(x,t) = k\mathrm{e}^{-\frac{p_0^2}{4\Delta^2}} \int_{-\infty}^{\infty} dp\ \mathrm{e}^{-\left[\frac{1}{4\Delta^2}+\frac{\mathrm{i}t}{2m\hbar}\right]p^2}\ \mathrm{e}^{\left[\frac{p_0}{2\Delta^2}+\frac{\mathrm{i}x}{\hbar}\right]p}$$
$$= k\sqrt{\frac{\pi}{\frac{1}{4\Delta^2}+\frac{\mathrm{i}t}{2m\hbar}}}\ \exp\left(\frac{\left[\frac{p_0}{2\Delta^2}+\frac{\mathrm{i}x}{\hbar}\right]^2}{\frac{1}{\Delta^2}+\frac{2\mathrm{i}t}{m\hbar}} - \frac{p_0^2}{4\Delta^2}\right)\,. \tag{2.48}$$

We are interested in particular in the x dependence of the probability density $\rho(x)$: that is solely related to the real part of the exponent of the rightmost term in (2.48), which can be expanded as follows:

$$\frac{\frac{p_0^2}{4\Delta^4}+\frac{\mathrm{i}p_0 x}{\Delta^2\hbar}-\frac{x^2}{\hbar^2}}{\frac{1}{\Delta^2}+\frac{2\mathrm{i}t}{m\hbar}} - \frac{p_0^2}{4\Delta^2} = -\frac{p_0^2}{4\Delta^2}\,\frac{\frac{4t^2\Delta^4}{m^2\hbar^2}+\frac{2\mathrm{i}t\Delta^2}{m\hbar}}{1+\frac{4t^2\Delta^4}{m^2\hbar^2}} - \left(\frac{\Delta^2 x^2}{\hbar^2} - \frac{\mathrm{i}p_0 x}{\hbar}\right)\frac{1-\frac{2\mathrm{i}t\Delta^2}{m\hbar}}{1+\frac{4t^2\Delta^4}{m^2\hbar^2}}$$

the real part being

$$-\frac{\Delta^2\left(x-\frac{p_0 t}{m}\right)^2}{\hbar^2\left(1+\frac{4t^2\Delta^4}{m^2\hbar^2}\right)} \equiv -\frac{\Delta^2\left(x-v_0 t\right)^2}{\hbar^2\left(1+\frac{4t^2\Delta^4}{m^2\hbar^2}\right)}\,.$$

Since p_0 is clearly the average momentum of the particle, we have introduced the corresponding average velocity $v_0 = p_0/m$. Recalling the definition of ρ as well as its normalization constraint, we finally find

$$\rho(x,t) = \frac{\Delta}{\hbar}\sqrt{\frac{2}{\pi\left(1+\frac{4t^2\Delta^4}{m^2\hbar^2}\right)}} \exp\left(-\frac{2\Delta^2}{\hbar^2}\frac{\left(x-v_0 t\right)^2}{1+\frac{4t^2\Delta^4}{m^2\hbar^2}}\right)\,, \tag{2.49}$$

while the probability distribution in terms of momentum reads

$$\tilde{\rho}(p) = \frac{1}{\sqrt{2\pi}\Delta}\mathrm{e}^{-(p-p_0)^2/(2\Delta^2)}\,. \tag{2.50}$$

Given a Gaussian distribution $\rho(x) = 1/(\sqrt{2\pi}\sigma)\mathrm{e}^{-(x-x_0)^2/(2\sigma^2)}$, it is a well known fact, which anyway can be easily derived from previous formulae, that the mean value $\bar{x}$ is x_0 while the mean quadratic deviation $\overline{(x-\bar{x})^2}$ is equal to σ^2. Hence, in the examined case, we have an average position $\bar{x} = v_0 t$ with a mean quadratic deviation equal to $\hbar^2/(4\Delta^2) + t^2\Delta^2/m^2$, while the average momentum is p_0 with a mean quadratic deviation Δ^2. The mean values represent the kinematic variables of a free particle, while the mean quadratic deviations are roughly inversely proportional to each other: if we improve the definition of one observable, the other becomes automatically less defined.

The distributions given in (2.49) and (2.50), even if derived in the context of a particular example, permit to reach important general conclusions which, for the sake of clarity, are listed in the following as distinct points.

2.4.1 The Uncertainty Principle

While the mean quadratic deviation relative to the momentum distribution

$$\overline{(p-\bar{p})^2} = \Delta^2$$

has been fixed a-priori by choosing $\tilde{\psi}(p)$ and is independent of time, thus confirming that momentum is a constant of motion for a free particle, that relative to the position

$$\overline{(x-\bar{x})^2} = \left(1 + \frac{4t^2\Delta^4}{m^2\hbar^2}\right)\frac{\hbar^2}{4\Delta^2}$$

does not contain further free parameters and does depend on time. Indeed, Δ_x grows significantly for $2t\Delta^2/(m\hbar) > 1$, hence for times greater than $t_s = m\hbar/(2\Delta^2)$. Notice that t_s is nothing but the time needed for a particle of momentum Δ to cover a distance $\hbar/(2\Delta)$, therefore this spreading has a natural interpretation also from a classical point of view: a set of independent particles having momenta distributed according to a width Δ_p, spreads with velocity $\Delta_p/m = v_s$; if the particles are statistically distributed in a region of size initially equal to Δ_x, the same size will grow significantly after times of the order of Δ_x/v_s.

What is new in our results is, first of all, that they refer to a single particle, meaning that uncertainties in position and momentum are not avoidable; secondly, these uncertainties are strictly interrelated. Without considering the spreading in time, it is evident that the uncertainty in one variable can be diminished only as the other uncertainty grows. Indeed, Δ can be eliminated from our equations by writing the inequality:

$$\Delta_x\Delta_p \equiv \sqrt{\overline{(x-\bar{x})^2}\;\overline{(p-\bar{p})^2}} \geq \frac{\hbar}{2}\,, \tag{2.51}$$

which is known as the *Heinsenberg uncertainty principle* and can be shown to be valid for any kind of wave packet. The case of a real Gaussian packet corresponds to the minimal possible value $\Delta_x\Delta_p = \hbar/2$.

From a phenomenological point of view this principle originates from the universality of diffractive phenomena. Indeed diffractive effects are those which prevent the possibility of a simultaneous measurement of position and momentum with arbitrarily good precision for both quantities. Let us consider for instance the case in which the measurement is performed through optical instruments; in order to improve the resolution it is necessary to make use of radiation of shorter wavelength, thus increasing the momenta of photons, which hitting the object under observation change its momentum in an unpredictable way. If instead position is determined through mechanical instruments, like slits, then the uncertainty in momentum is caused by diffractive phenomena.

It is important to evaluate the order of magnitude of quantum uncertainty in cases of practical interest. Let us consider for instance a beam of electrons emitted by a cathode at a temperature $T = 1000°$K and accelerated through a potential difference equal to 10^4 V. The order of magnitude of the kinetic energy uncertainty Δ_E is kT, where $k = 1.381\ 10^{-23}$ J/°K is the Boltzmann constant (alternatively one can use $k = 8.617\ 10^{-5}$ eV/°K). Therefore $\Delta_E = 1.38\ 10^{-20}$ J while $E = 1.6\ 10^{-15}$ J, corresponding to a quite precise determination of the beam energy ($\Delta_E/E \sim 10^{-5}$). We can easily compute the momentum uncertainty by using error propagation ($\Delta_p/p = \frac{1}{2}\Delta_E/E$) and computing $p = \sqrt{2m_eE} = 5.6\ 10^{-23}$ N s; we thus obtain $\Delta_p = 2.8\ 10^{-28}$ N s, hence, making use of (2.51), $\Delta_x \geq 2\ 10^{-7}$ m. It is clear that the uncertainty principle does not place significant constraints in the case of particle beams.

A macroscopic body of mass $M = 1$ Kg placed at room temperature ($T \simeq 300°$K) has an average thermal momentum , caused by collisions with air molecules, which is equal to $\Delta_p \sim \sqrt{2M\ 3kT/2} \simeq 9\ 10^{-11}$ N s, so that the minimal quantum uncertainty on its position is $\Delta_x \sim 10^{-24}$ m, hence not appreciable.

The uncertainty principle is instead quite relevant at the atomic level, where it is the stabilizing mechanism which prevents the electron from collapsing onto the nucleus. We can think of the electron orbital radius as a rough estimate of its position uncertainty ($\Delta_x \sim r$) and evaluate the kinetic energy deriving from the momentum uncertainty; we have $E_k \sim \Delta_p^2/(2m) \sim \hbar^2/(2mr^2)$. Taking into account the binding Coulomb energy, the total energy is

$$E(r) \sim \frac{\hbar^2}{2mr^2} - \frac{e^2}{4\pi\epsilon_0 r}\,.$$

We infer that the system is stable, since the total energy $E(r)$ has an absolute minimum. The stable radius r_m corresponding to this minimum can be computed through the equation

$$\frac{e^2}{4\pi\epsilon_0 r_m^2} - \frac{\hbar^2}{m r_m^3} = 0\,,$$

hence

$$r_m \sim \frac{4\pi\epsilon_0\hbar^2}{me^2} ,$$

which nicely reproduce the value of the atomic radius for the fundamental level in Bohr's model, see (2.22).

2.4.2 The Speed of Waves

It is known that electromagnetic waves move without distortion at a speed $c = 1/\sqrt{\epsilon_0\mu_0}$ and that, for a harmonic wave, c is given by the wavelength multiplied by the frequency.

In the case of de Broglie's waves introduced in (2.40), we have $\nu = p^2/(2mh)$ and $\lambda = h/p$; therefore the velocity of harmonic waves is given by $v_F \equiv \lambda\nu = p/(2m)$. If we consider instead the wave packet given in (2.48) and its corresponding probability density given in (2.49), we clearly see that it moves with a velocity $v_G \equiv p_0/m$, which is equal to the classical velocity of a particle with momentum p_0. We have used different symbols to distinguish the velocity of plane waves v_F, which is called *phase velocity*, from v_G, which is the speed of the packet and is called *group velocity*. Previous equations lead to the result that, contrary to what happens for electromagnetic waves propagating in vacuum, the two velocities are different for de Broglie's waves, and in particular the group velocity does not coincide with the average value of the phase velocities of the different plane waves making up the packet. Moreover, the phase velocity depends on the wavelength ($v_F = h/(2m\lambda)$). The relation between frequency and wavelength is given by $\nu = c/\lambda$ for electromagnetic waves, while for de Broglie's waves it is $\nu = h/(2m\lambda^2)$.

There is a very large number of examples of wave-like propagation in physics: electromagnetic waves, elastic waves, gravity waves in liquids and several other ones. In each case the frequency presents a characteristic dependence on the wavelength, $\nu(\lambda)$. Considering as above the propagation of gaussian wave packets, it is always possible to define the phase velocity, $v_F = \lambda\ \nu(\lambda)$, and the group velocity, which in general is defined by the relation:

$$v_G = -\lambda^2 \frac{d\nu(\lambda)}{d\lambda} . \qquad (2.52)$$

Last equation can be verified by considering that, for a generic dependence of the wave phase on the wave number $\exp(\mathrm{i}kx - \mathrm{i}\omega(k)t)$ and for a generic wave packet described by superposition coefficients strongly peaked around a given value $k = k_0$, the resulting wave function

$$\psi(x) \propto \int_{-\infty}^{\infty} dk\ f(k-k_0)\ \mathrm{e}^{\mathrm{i}(kx-\omega(k)t)} .$$

will be peaked around an x_0 such that the phase factor is stationary, hence almost constant, for $k \sim k_0$, leading to $x_0 \sim \omega'(k_0)t$.

In the case of de Broglie's waves (2.52) reproduces the result found previously. Media where the frequency is inversely proportional to the wavelength, as for electromagnetic waves in vacuum, are called *non-dispersive media*, and in that case the two velocities coincide.

It may be interesting to notice that, if we adopt the relativistic form for the plane wave, we have $\nu(\lambda) = \sqrt{m^2c^4/h^2 + c^2/\lambda^2}$, hence

$$v_F = \lambda\sqrt{\frac{m^2c^4}{h^2} + \frac{c^2}{\lambda^2}} = \frac{E}{p} > c\,,$$

$$v_G = \frac{c^2}{\lambda}\left(\frac{m^2c^4}{h^2} + \frac{c^2}{\lambda^2}\right)^{-1/2} = \frac{pc^2}{E} < c\,.$$

In particular v_G, which describes the motion of wave packets, satisfies the constraint of being less than c and coincides with the relativistic expression for the speed of a particle in terms of momentum and energy given in Chapter 1.

2.4.3 The Collective Interpretation of de Broglie's Waves

The description of single particles as wave packets is at the basis of a rigorous formulation of Schrödinger's theory. There is however an alternative interpretation of the wave function, which is of much simpler use and can be particularly useful to describe average properties, like a particle flow in the free case.

Let us consider the plane wave in (2.40): $\psi = \exp\left(\mathrm{i}\left(p\,x - p^2t/(2m)\right)/\hbar\right)$ and compute the corresponding current density J:

$$J = -\frac{\mathrm{i}\hbar}{2m}\left(\psi^*\partial_x\psi - \psi\partial_x\psi^*\right) = -\frac{\mathrm{i}\hbar}{2m}\left(\psi^*\frac{\mathrm{i}p}{\hbar}\psi - \psi\frac{-\mathrm{i}p}{\hbar}\psi^*\right) = \frac{p}{m}\,, \qquad (2.53)$$

while $\rho = \psi^*\psi = 1$. On the other hand we notice that given a distribution of classical particles with density ρ and moving with velocity v, the corresponding current density is $J = \rho v$.

That suggests to go beyond the problem of normalizing the probability distribution in (2.44), relating instead the wave function in (2.40) not to a single particle, as we have done till now, but to a stationary flux of independent particles, which are uniformly distributed with unitary density and move with the same velocity v.

It should be clear that in this way we are a priori giving up the idea of particle localization, however we obtain in a much simpler way information about the group velocity and the flux. We will thus be able, in the following Chapter, to easily and clearly interpret the effects of a potential barrier on a particle flux.

2.5 The Potential Barrier

The most interesting physical situation is that in which particles are not free, but subject to forces corresponding to a potential energy $V(x)$. In these conditions the Schrödinger equation in the form given in (2.42) has to be used. Since the equation is linear, the study can be limited, without loss of generality, to solutions which are periodic in time, like:

$$\psi(x,t) = \mathrm{e}^{-\mathrm{i}Et/\hbar}\psi_E(x)\,. \tag{2.54}$$

Indeed the general time dependent solution can always be decomposed in periodic components through a Fourier expansion, so that its knowledge is equivalent to that of $\psi_E(x)$ plus the expansion coefficients.

Furthermore, according to the collective interpretation of de Broglie waves presented in last Section, the wave function in (2.54) describes either a stationary flow or a stationary state of particles. In particular we shall begin studying a stationary flow hitting a potential barrier.

The function $\psi_E(x)$ is a solution of the equation obtained by replacing (2.54) into (2.42), i.e.

$$\mathrm{i}\hbar\ \partial_t \mathrm{e}^{-\mathrm{i}Et/\hbar}\psi_E(x) = E\mathrm{e}^{-\mathrm{i}Et/\hbar}\psi_E(x) = \mathrm{e}^{-\mathrm{i}Et/\hbar}\left[-\frac{\hbar^2}{2m}\partial_x^2\psi_E + V(x)\psi_E\right] \tag{2.55}$$

hence

$$E\psi_E(x) = -\frac{\hbar^2}{2m}\partial_x^2\psi_E(x) + V(x)\psi_E(x)\,, \tag{2.56}$$

which is known as the *time-independent* or *stationary* schrödinger equation.

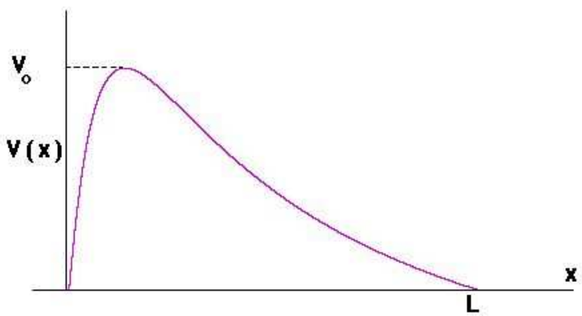
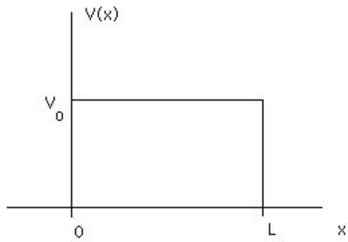


Fig. 2.3. A typical example of a potential barrier, referring in particular to that due to Coulomb repulsion that will be used when discussing Gamow's theory of nuclear α-emission

We will consider at first the case of a *potential barrier*, in which $V(x)$ vanishes for $x < 0$ and $x > L$, and is positive in the segment $[0, L]$, as shown in Fig. 2.3. A flux of classical particles hitting the barrier from the left will experience slowing forces as $x > 0$. If the starting kinetic energy, corresponding in this case to the total energy E in (2.56), is greater than the barrier height V_0, the particles will reach the point where V has a maximum, being accelerated from there forward till they pass point $x = L$, where the motion gets free again. Therefore the flux is completely transmitted, the effect of the barrier being simply a slowing down in the segment $[0, L]$. If instead the kinetic energy is less than V_0, the particles will stop before they reach the point where V has a maximum, reversing their motion afterwards: the flux is completely reflected in this case. Quantum Mechanics gives a completely different result.

In order to analyze the differences from a qualitative point of view, it is convenient to choose a barrier which makes the solution of (2.56) easier: that is the case of a potential which is piecewise constant, like the square barrier depicted on the side. The choice is motivated by the fact that, if V is constant, then (2.56) can be rewritten as follows:



$$\partial_x^2 \psi_E(x) + \frac{2m}{\hbar^2}(E - V)\psi_E(x) = 0\,, \tag{2.57}$$

and has the general solution:

$$\psi_E(x) = a_+ \exp\left(\mathrm{i}\frac{\sqrt{2m(E-V)}}{\hbar}x\right) + a_- \exp\left(-\mathrm{i}\frac{\sqrt{2m(E-V)}}{\hbar}x\right)\,, \tag{2.58}$$

if $E > V$, while

$$\psi_E(x) = a_+ \exp\left(\frac{\sqrt{2m(V-E)}}{\hbar}x\right) + a_- \exp\left(-\frac{\sqrt{2m(V-E)}}{\hbar}x\right)\,, \tag{2.59}$$

in the opposite case. The problem is then to establish how the solution found in a definite region can be connected to those found in the nearby regions. In order to solve this kind of problem we must be able to manage differential equations in presence of discontinuities in their coefficients, and that requires a brief *mathematical interlude.*

2.5.1 Mathematical Interlude: Differential Equations with Discontinuous Coefficients

Differential equations with discontinuous coefficients can be treated by smoothing the discontinuities, then solving the equations in terms of functions which are derivable several times, and finally reproducing the correct solutions in presence of discontinuities through a limit process. In order to do so, let us introduce the function $\varphi_\epsilon(x)$, which is defined as

$$\varphi_\epsilon(x) = 0 \quad \text{if} \quad |x| > \epsilon\,,$$

$$\varphi_\epsilon(x) = \frac{\epsilon^2 + x^2}{2\left(\epsilon^2 - x^2\right)^2} \frac{1}{\cosh^2\left(x/(\epsilon^2 - x^2)\right)} \quad \text{if} \quad |x| < \epsilon\,.$$

This function, as well as all of its derivatives, is continuous and it can be easily shown that

$$\int_{-\infty}^{\infty} \varphi_\epsilon(x) dx = 1\,.$$

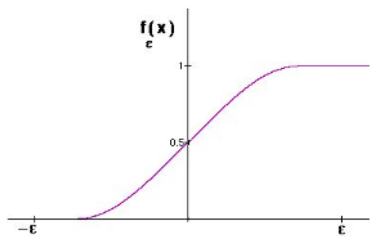
Based on this property we conclude that if $f(x)$ is locally integrable, i.e. if it admits at most isolated singularities where the function may diverge with a degree less than one, like for instance $1/|x|^{1-\delta}$ when $\delta > 0$, then the integral

$$\int_{-\infty}^{\infty} \varphi_\epsilon(x-y) f(y) dy \equiv f_\epsilon(x)$$

defines a function which can be derived in x an infinite number of times; the derivatives of f_ϵ tend to those of f in the limit $\epsilon \to 0$ and in all points where the latter are defined. We have in particular, by part integration,

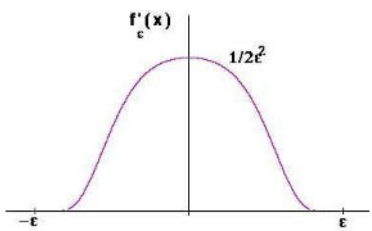
$$\frac{d^n}{dx^n} f_\epsilon(x) = \int_{-\infty}^{\infty} \varphi_\epsilon(x-y) \frac{d^n}{dy^n} f(y) dy\,. \tag{2.60}$$

f_ϵ is called *regularized function*. If for instance we consider the case in which f is the step function in the origin, i.e. $f(x) = 0$ for $x < 0$ and $f(x) = 1$ for $x > 0$, we have for $f_\epsilon(x)$, $\partial_x f_\epsilon(x) = f'_\epsilon(x)$ and $\partial_x^2 f_\epsilon(x) = f''_\epsilon(x)$ the behaviours showed in the respective order on the side. Notice in particular that since

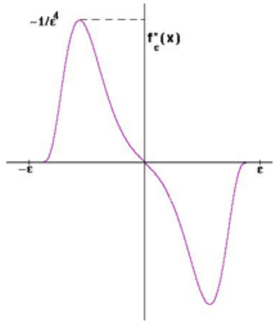


$$f_\epsilon(x) = \int_0^{\infty} \varphi_\epsilon(x-y) dy = \int_{-\infty}^{x} \varphi_\epsilon(z) dz$$

we have $\partial_x f_\epsilon(x) = \varphi_\epsilon(x)$. By looking at the three figures it is clear that $f_\epsilon(x)$ continuously interpolates between the two values, zero and one, which the function assumes respectively to the left of $-\epsilon$ and to the right of ϵ, staying less than 1 for every value of x. It is important to notice that instead the second figure, showing $\partial_x f_\epsilon(x)$, i.e. $\varphi_\epsilon(x)$, has a maximum of height proportional to $1/\epsilon^2$, hence diverging as $\epsilon \to 0$.



The third figure, showing the second derivative $\partial_x^2 f_\epsilon(x)$, has an oscillation of amplitude proportional to $1/\epsilon^4$ around the discontinuity point. Since, for small ϵ, the regularized function depends, close to the discontinuity, on the nearby values of the original function, it is clear that the qualitative behaviors showed in the figures are valid, close to discontinuities of the first kind (i.e. where the function itself has a discontinuous gap), for every starting function f.



Let us now consider (2.57) close to a discontinuity point of the first kind (step function) for V, and suppose we regularize both terms on the left hand side. Assuming that the wave function do not present discontinuities worse than first kind, the second term in the equation may present only steps so that, once regularized, it is limited independently of ϵ. However the first term may present oscillations of amplitude $\sim 1/\epsilon^4$ if ψ_E has a first kind discontinuity, or a peak of height $\sim \pm 1/\epsilon^2$ if ψ_E is continuous but its first derivative has such discontinuity: in each case the modulus of the first regularized term would diverge faster than the second in the limit $\epsilon \to 0$. That shows that in presence of a first kind discontinuity in V, both the wave function ψ_E and its derivative must be continuous.

In order to simply deal with barriers of length L much smaller than the typical wavelengths of the problem, it is useful to introduce infinitely thin barriers: that can be done by choosing a potential energy which, once regularized, be equal to $V_\epsilon(x) = \mathcal{V}\ \varphi_\epsilon(x)$, i.e.

$$V(x) = \mathcal{V} \lim_{\epsilon \to 0} \varphi_\epsilon(x) \equiv \mathcal{V}\delta(x)\,. \tag{2.61}$$

Equation (2.61) defines the so-called *Dirac's delta function* as a limit of φ_ϵ.

When studying Schrödinger equation regularized as done above, it is possible to show, by integrating the differential equation between $-\epsilon$ and ϵ, that in presence of a potential barrier proportional to the Dirac delta function the wave function stays continuous but its derivative has a first kind discontinuity of amplitude

$$\lim_{\epsilon \to 0}(\psi'_E(\epsilon) - \psi'_E(-\epsilon)) = \frac{2m}{\hbar^2}\mathcal{V}\psi_E(0)\,. \tag{2.62}$$

Notice that a potential barrier proportional to the Dirac delta function can be represented equally well by a square barrier of height $\mathcal{V}/L$ and width L, in the limit as $L \to 0$ with $\int_{-\infty}^{\infty} dx V(x) = \mathcal{V}$ kept constant.

2.5.2 The Square Barrier

Let us consider the stationary Schrödinger equation (2.56) with a potential corresponding to the square barrier described above, that is $V(x) = V$ for