Recapitulación

$\hat{H}$ independiente de t

$\hat{H}|\varphi_n\rangle = E_n|\varphi_n\rangle$

$$|\Psi(0)\rangle = \sum_n C_n(0)\,|\varphi_n\rangle \rightarrow |\Psi(t)\rangle = \sum_n C_n(0)\, e^{-iE_nt/\hbar}\,|\varphi_n\rangle$$

Es importante resolver $\hat{H}|\varphi_n\rangle = E_n|\varphi_n\rangle$

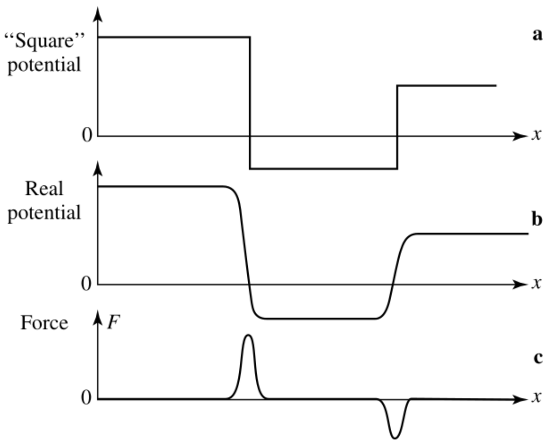
En la representación $\{|\vec{r}\rangle\}$, para $\hat{H} = \frac{\hat{P}^2}{2m} + V(\hat{\vec{R}})$

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\varphi(\vec{r}) = E\,\varphi(\vec{r})$$

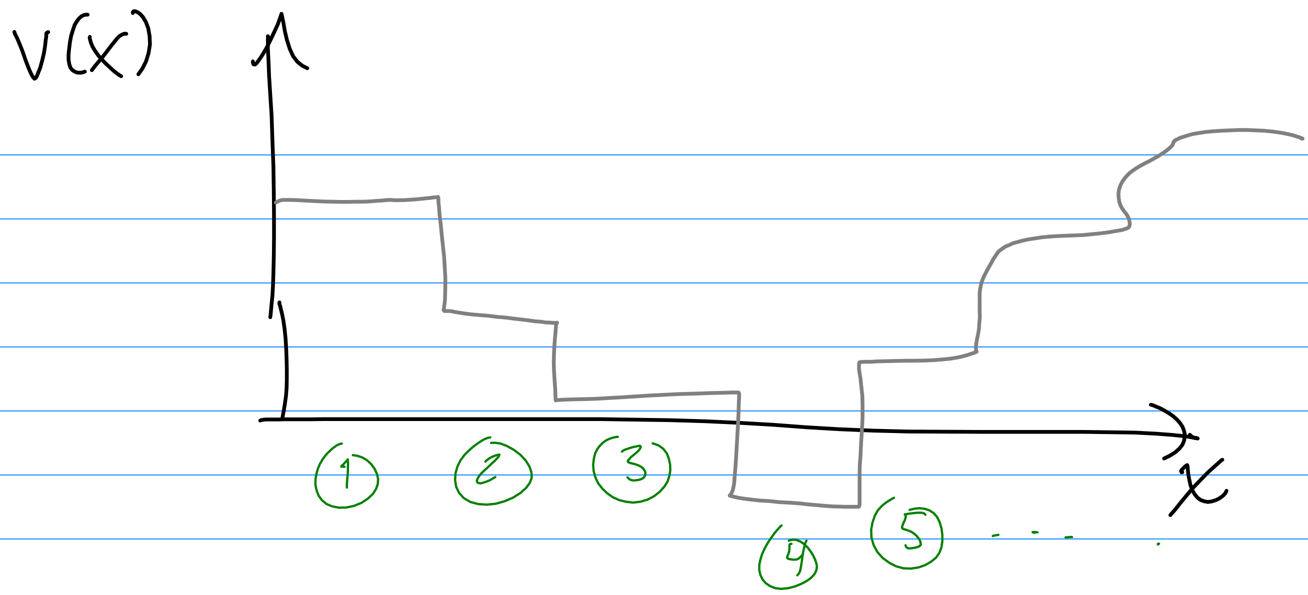
Potenciales cuadrados. (1D)

1. Son fáciles de resolver (para empezar)
2. Similar a óptica, los efectos cuánticos aparecen cuando el potencial varía en distancias cortas comparado con $\lambda = \frac{h}{p}$

C T I H_I



$F = -\frac{dV}{dx}$



1. Behavior of a stationary wave function $\varphi(x)$

1-a. Regions of constant potential energy

In the case of a square potential, $V(x)$ is a constant function $V(x) = V$ in certain regions of space. In such a region, equation (D-8) of Chapter I can be written:

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\varphi(x) + \frac{2m}{\hbar^2}(E - V)\,\varphi(x) = 0 \tag{1}$$

We shall distinguish between several cases:

(*i*) $E > V$
Let us introduce the positive constant k, defined by

$$E - V = \frac{\hbar^2 k^2}{2m} \tag{2}$$

The solution of equation (1) can then be written:

$$\varphi(x) = A\,\mathrm{e}^{ikx} + A'\,\mathrm{e}^{-ikx} \tag{3}$$

where A and A' are complex constants.

(*ii*) $E < V$
This condition corresponds to regions of space which would be forbidden to the particle by the laws of classical mechanics. In this case, we introduce the positive constant ρ defined by:

$$V - E = \frac{\hbar^2 \rho^2}{2m} \tag{4}$$

and the solution of (1) can be written:

$$\varphi(x) = B\,\mathrm{e}^{\rho x} + B'\,\mathrm{e}^{-\rho x} \tag{5}$$

where B and B' are complex constants.

(*iii*) $E = V$. In this special case, $\varphi(x)$ is a linear function of x.

1-b. Behavior of $\varphi(x)$ at a potential energy discontinuity

How does the wave function behave at a point $x = x_1$, where the potential $V(x)$ is discontinuous? One might expect the wave function $\varphi(x)$ to behave strangely at this point, becoming itself discontinuous, for example. The aim of this section is to show that this is not the case: $\varphi(x)$ and $\mathrm{d}\varphi/\mathrm{d}x$ are continuous, and it is only the second derivative $\mathrm{d}^2\varphi/\mathrm{d}x^2$ that is discontinuous at $x = x_1$.

Without giving a rigorous proof, let us try to understand this property. To do this, recall that a square potential must be considered (*cf.* Chap. I, § D-2-a) as the limit, when $\varepsilon \longrightarrow 0$, of a potential $V_\varepsilon(x)$ equal to $V(x)$ outside the interval $[x_1 - \varepsilon, x_1 + \varepsilon]$, and varying continuously within this interval. Then consider the equation:

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\varphi_\varepsilon(x) + \frac{2m}{\hbar^2}[E - V_\varepsilon(x)]\varphi_\varepsilon(x) = 0 \tag{6}$$

where $V_\varepsilon(x)$ is assumed to be bounded, independently of ε, within the interval $[x_1 - \varepsilon, x_1 + \varepsilon]$. Choose a solution $\varphi_\varepsilon(x)$ which, for $x < x_1 - \varepsilon$, coincides with a given solution of (1). The problem is to show that, when $\varepsilon \longrightarrow 0$, $\varphi_\varepsilon(x)$ tends towards a function $\varphi(x)$ which is continuous and differentiable at $x = x_1$. Let us grant that $\varphi_\varepsilon(x)$ remains bounded[1], whatever the value of ε, in the neighborhood of $x = x_1$. Physically, this means that the probability density remains finite. Integrating (6) between $x_1 - \eta$ and $x_1 + \eta$, we obtain:

por propiedades de ecs. dif.

$$\frac{\mathrm{d}\varphi_\varepsilon}{\mathrm{d}x}(x_1 + \eta) - \frac{\mathrm{d}\varphi_\varepsilon}{\mathrm{d}x}(x_1 - \eta) = \frac{2m}{\hbar^2}\int_{x_1-\eta}^{x_1+\eta} [V_\varepsilon(x) - E]\,\varphi_\varepsilon(x)\,\mathrm{d}x \tag{7}$$

At the limit where $\varepsilon \longrightarrow 0$, the function to be integrated on the right-hand side of this expression remains bounded, owing to our previous assumption. Consequently, if η tends towards zero, the integral also tends towards zero, and:

$$\frac{\mathrm{d}\varphi}{\mathrm{d}x}(x_1 + \eta) - \frac{\mathrm{d}\varphi}{\mathrm{d}x}(x_1 - \eta) \underset{\eta \to 0}{\longrightarrow} 0 \tag{8}$$

(como la derivada es continua la función también)

Thus, at this limit, $\mathrm{d}\varphi/\mathrm{d}x$ is continuous at $x = x_1$, and so is $\varphi(x)$ (since it is the integral of a continuous function). On the other hand, $\mathrm{d}^2\varphi/\mathrm{d}x^2$ is discontinuous, and, as can be seen directly from (1), makes a jump at $x = x_1$, which is equal to $\frac{2m}{\hbar^2}\varphi(x_1)\,\sigma_V$ [where σ_V represents the change in $V(x)$ at $x = x_1$].

Comment:

It is essential, in the preceding argument, that $V_\varepsilon(x)$ remain bounded. In certain exercises of Complement $\mathrm{K_I}$, for example, the case is considered for which $V(x) = \alpha\,\delta(x)$, an unbounded function whose integral remains finite. In this case, $\varphi(x)$ remains continuous, but $\mathrm{d}\varphi/\mathrm{d}x$ does not.

1-c. Outline of the calculation

The procedure for determining the stationary states in a "square potential" is therefore the following: in all regions where $V(x)$ is constant, write $\varphi(x)$ in whichever of the two forms (3) or (5) is applicable; then "match" these functions by requiring the continuity of $\varphi(x)$ and of $\mathrm{d}\varphi/\mathrm{d}x$ at the points where $V(x)$ is discontinuous.