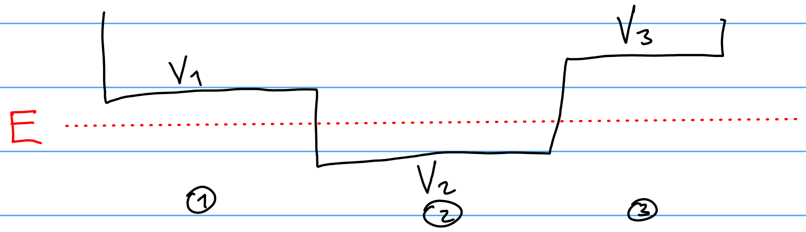
Recapitulación

Potenciales constantes por pedazos.

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



1) Dividir el problema en regiones const.

2) Resolver la ec. de Schrödinger en cada región.

Para $E > V_j$: $E - V_k = \frac{\hbar^2 k_j^2}{2m}$ $\varphi_j(x) = A_j e^{ik_j x} + A_j' e^{-ik_j x}$

Para $E < V_j$: $V_k - E = \frac{\hbar^2 \rho_j^2}{2m}$ $\varphi_j(x) = B_j e^{\rho x} + B_j' e^{-\rho x}$

Para $E = V_j$: $\varphi_j(x) = Cx + D$

3) Pegar las soluciones.

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:

$$\frac{\mathrm{d}\varphi}{\mathrm{d}x}(x_1 + \eta) - \frac{\mathrm{d}\varphi}{\mathrm{d}x}(x_1 - \eta) \xrightarrow[\eta \to 0]{} 0 \tag{8}$$

(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.

Un resultado útil.

complement

E debe ser $> \min(V(x))$ CT III M_{III}

$\hat{H} = \hat{T} + \hat{V}$ si $\hat{H}|\varphi\rangle = E|\varphi\rangle$

mult por $\langle\varphi|$

$$\langle\varphi|\hat{H}|\varphi\rangle = E \cancel{\langle\varphi|\varphi\rangle}^{1}$$

$$\langle\hat{T}\rangle + \langle\hat{V}\rangle = E$$

$$\langle T\rangle = \frac{1}{2m}\langle\hat{p}^2\rangle = \int p^2 |\varphi(p)|^2 dp \geq 0$$

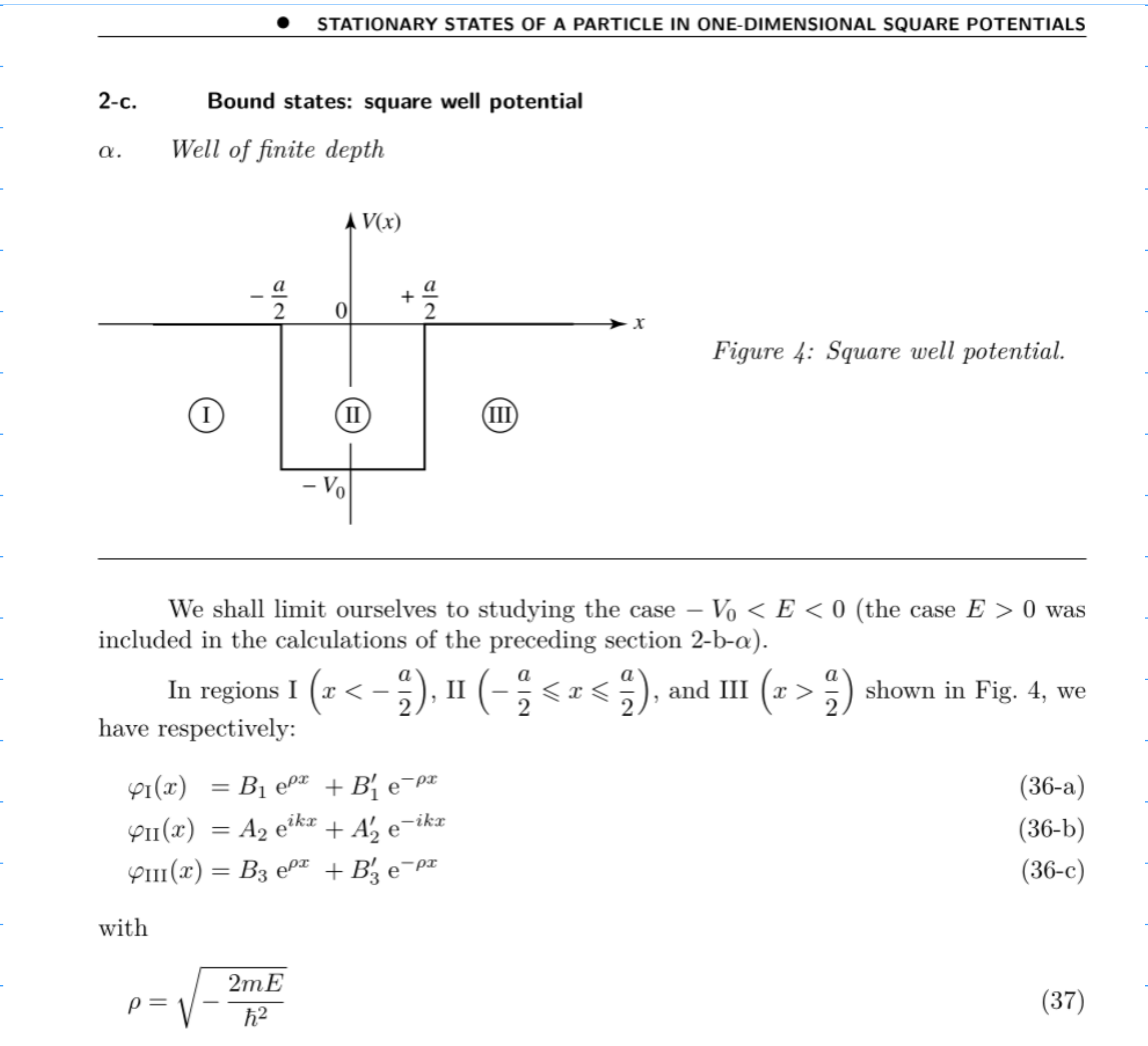
$$\langle V\rangle = \int V(x)|\varphi(x)|^2 dx \geq \int(-V_0)\,|\varphi(x)|^2 dx \geq -V_0 = (\min V(x))$$

$$E = \langle\hat{T}\rangle + \langle\hat{V}\rangle \geq \langle\hat{V}\rangle \geq -V_0$$

Comentar que $E_{min} > \min(V(x))$

Pozo cuadrado

CT I H_I



2-c. **Bound states: square well potential**

α. *Well of finite depth*

Figure 4: Square well potential.

We shall limit ourselves to studying the case $-V_0 < E < 0$ (the case $E > 0$ was included in the calculations of the preceding section 2-b-α).

In regions I $\left(x < -\frac{a}{2}\right)$, II $\left(-\frac{a}{2} \leqslant x \leqslant \frac{a}{2}\right)$, and III $\left(x > \frac{a}{2}\right)$ shown in Fig. 4, we have respectively:

$$\varphi_{\mathrm{I}}(x) = B_1\, \mathrm{e}^{\rho x} + B_1'\, \mathrm{e}^{-\rho x} \tag{36-a}$$

$$\varphi_{\mathrm{II}}(x) = A_2\, \mathrm{e}^{ikx} + A_2'\, \mathrm{e}^{-ikx} \tag{36-b}$$

$$\varphi_{\mathrm{III}}(x) = B_3\, \mathrm{e}^{\rho x} + B_3'\, \mathrm{e}^{-\rho x} \tag{36-c}$$

with

$$\rho = \sqrt{-\frac{2mE}{\hbar^2}} \tag{37}$$

Queda encontrar la relación entre ρ, k y las otras constantes para satisfacer las condiciones de frontera.