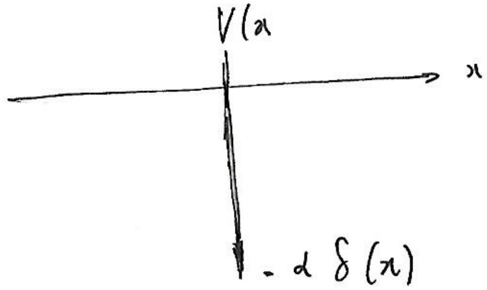
Potenciais tipo delta de Dirac



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

contorno: $\psi(x)$ contínua $\qquad \psi(\pm\infty) = 0$

$$\lim_{\varepsilon\to 0}\left\{-\frac{\hbar^2}{2m}\int_{-\varepsilon}^{\varepsilon}\frac{d^2\psi}{dx^2}\,dx + \int_{-\varepsilon}^{\varepsilon}V(x)\,\psi(x) = E\,\cancel{\int_{-\varepsilon}^{\varepsilon}\underbrace{\psi(x)}_{\text{contínua}}\,dx}^{\,0}\right\}$$

$$\lim_{\varepsilon\to 0}\left\{\left.\frac{d\psi}{dx}\right|_{\varepsilon} - \left.\frac{d\psi}{dx}\right|_{-\varepsilon} = \frac{2m}{\hbar^2}\int_{-\varepsilon}^{\varepsilon}V(x)\,\psi(x)\,dx\right\} \implies \frac{d\psi}{dx} \text{ contínua}$$

p/ potenciais contínuos ou singularidades removíveis

p/ potenciais tipo delta: $V(x) = -\alpha\,\delta(x)$ $\implies$ $\boxed{\left.\frac{d\psi}{dx}\right|_{0^+} - \left.\frac{d\psi}{dx}\right|_{0^-} = -\frac{2m\alpha}{\hbar^2}\psi(0)}$

Estados ligados: $E<0$

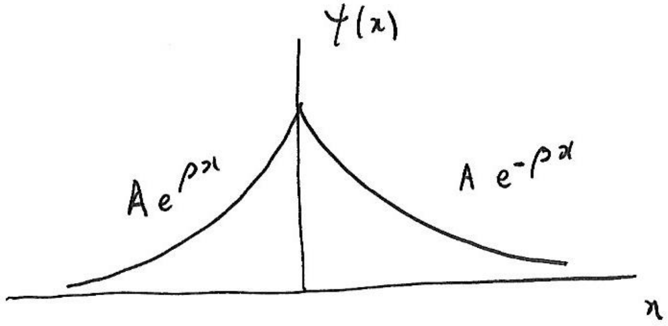
$\delta(x)$ - par $\implies$ $\psi(x)$ - paridade definida

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi = -|E|\psi \implies \frac{d^2\psi}{dx^2} - \underbrace{\left(\frac{2m|E|}{\hbar^2}\right)}_{\rho^2}\psi = 0 \quad \left(\begin{matrix} x<0 \\ \text{e} \\ x>0\end{matrix}\right)$$

$A\,e^{\rho x} \to 0 \quad (x \to -\infty)$

$B\,e^{-\rho x} \to 0 \quad (x \to \infty)$

$\psi(0^+) = \psi(0^-) \implies B = A$



$$\rho^2 = \frac{2m|E|}{\hbar^2} \qquad \psi(x) = A e^{-\rho|x|}$$

normalização :

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 2A^2 \underbrace{\int_0^{\infty} e^{-2\rho x} dx}_{\frac{1}{2\rho} e^{-2\rho x}\Big|_{\infty}^{0} = \frac{1}{2\rho}} = 1 \implies \boxed{A = \sqrt{\rho}}$$

$$\begin{cases} \left.\dfrac{d\psi}{dx}\right|_{0^+} = -\rho A \\ \left.\dfrac{d\psi}{dx}\right|_{0^-} = \rho A \end{cases} \implies -2\rho = -\frac{2m\alpha}{\hbar^2} \implies \rho = \frac{m\alpha}{\hbar^2} \implies \begin{cases} A = \dfrac{\sqrt{m\alpha}}{\hbar} \\ |E| = \dfrac{m\alpha^2}{2\hbar^2} \end{cases}$$

único estado ligado

$$\begin{cases} \psi(x) = \dfrac{\sqrt{m\alpha}}{\hbar} e^{-\frac{m\alpha}{\hbar^2}|x|} \\ E = -\dfrac{m\alpha^2}{2\hbar^2} \end{cases}$$

Estados não-ligados : $E > 0$ $\longrightarrow$ (incidência)

$$\begin{cases} \psi(x<0) = A e^{ikx} + B e^{-ikx} \\ \psi(x>0) = C e^{ikx} \end{cases} \qquad \left(k = \frac{\sqrt{2mE}}{\hbar}\right) \qquad -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \Rightarrow \frac{d^2\psi}{dx^2} + \underbrace{\left(\frac{2mE}{\hbar^2}\right)}_{k^2}\psi = 0$$

contorno
$$\begin{cases} \psi(x) \text{ contínua} \Rightarrow A + B = C \\ \left.\frac{d\psi}{dx}\right|_{0^+} - \left.\frac{d\psi}{dx}\right|_{0^-} = -\frac{2m\alpha}{\hbar^2}\psi(0) \Rightarrow ik(C - A + B) = -\frac{2m\alpha}{\hbar^2} C \Rightarrow C - (A-B) = i\frac{2m\alpha}{\hbar^2 k} C \end{cases}$$

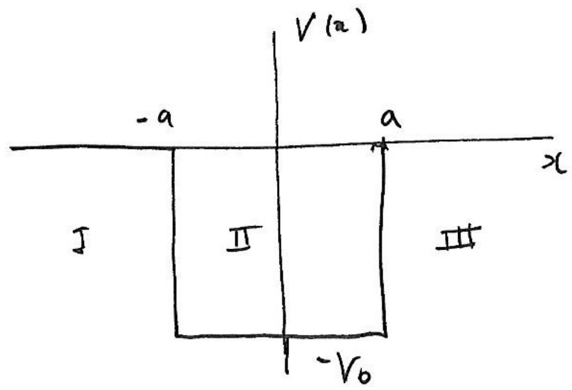
$$A + B = C$$
$$A - B = \left(1 - i\frac{2m\alpha}{\hbar^2 k}\right) C$$
$$\overline{\qquad\qquad\qquad\qquad}$$
$$2A = \left(2 - i\frac{2m\alpha}{\hbar^2 k}\right) C \Longrightarrow \frac{C}{A} = \frac{1}{1 - i\frac{m\alpha}{\hbar^2 k}} \Rightarrow T = \left|\frac{C}{A}\right|^2 = \frac{1}{1 + \left(\frac{m\alpha}{\hbar^2 k}\right)^2}$$

coeficiente de transmissão
$$\boxed{T = \frac{1}{1 + m\alpha^2/2\hbar^2 E}} \Rightarrow R = 1 - T = \frac{1 + m\alpha^2/2\hbar^2E - 1}{1 + m\alpha^2/2\hbar^2 E}$$

coeficiente de reflexão
$$\boxed{R = \frac{1}{1 + 2\hbar^2 E/m\alpha^2}}$$

Poço retangular finito

$$V(x) = \begin{cases} 0 & (|x| > a) \\ -V_0 & (-a < x < a) \end{cases}$$



Estados ligados : $-V_0 < E < 0$

região I : $x < -a$ $\Rightarrow$ $-\frac{\hbar^2}{2m}\frac{d^2\psi_I}{dx^2} = -|E|\psi_I$ $\Rightarrow$ $\frac{d^2\psi_I}{dx^2} = \underbrace{\left(\frac{2m|E|}{\hbar^2}\right)}_{\rho^2}\psi_I$.

(V = 0)

$\boxed{\psi_I = B\,e^{\rho x}} \to 0 \ (x \to -\infty)$ $\qquad \rho = \frac{\sqrt{2m|E|}}{\hbar}$

região II : $-a < x < a$ $\Rightarrow$ $-\frac{\hbar^2}{2m}\frac{d^2\psi_{II}}{dx^2} - V_0\psi_{II} = -|E|\psi_{II}$ $\Rightarrow$ $\frac{d^2\psi_{II}}{dx^2} + \underbrace{\frac{2m(V_0-|E|)}{\hbar^2}}_{k^2}\psi_{II} = 0$

($V = -V_0$)

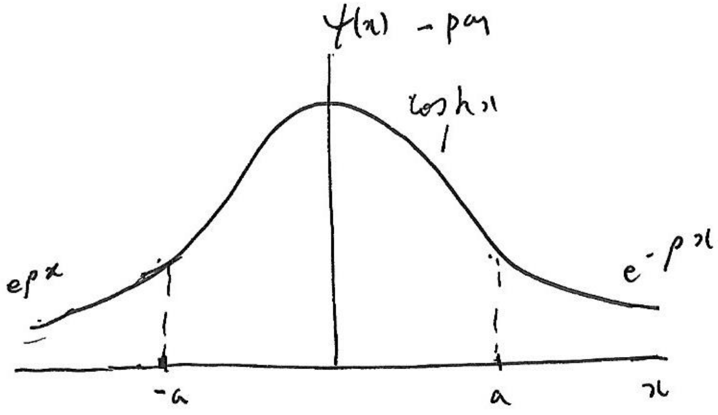
$\boxed{\psi_{II} = C\sin kx + D\cos kx}$ $\qquad k = \frac{\sqrt{2m(V_0-|E|)}}{\hbar}$ $\qquad \boxed{\rho^2 + k^2 = \frac{2mV_0}{\hbar^2}}$

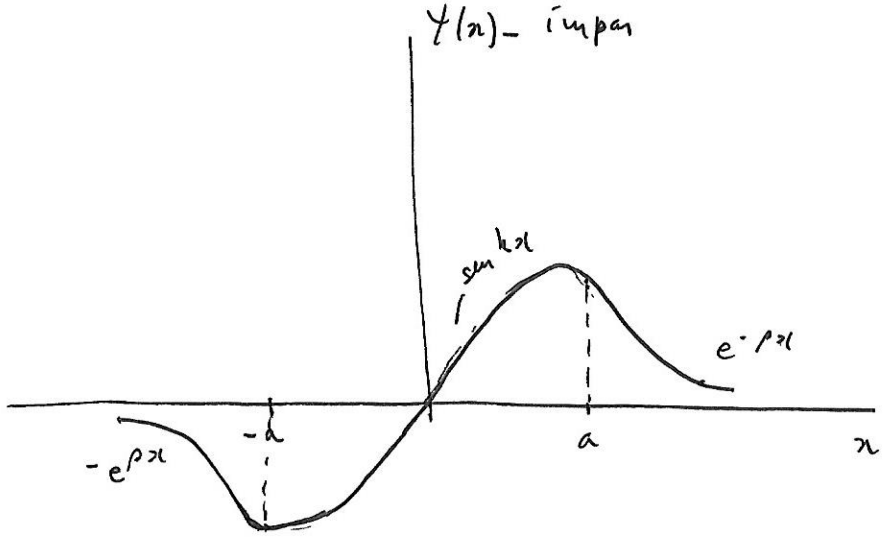
região III : $x > a$ $\Rightarrow$ $\frac{d^2\psi_{III}}{dx^2} = \rho^2\psi_{III}$

(V = 0)

$\boxed{\psi_{III} = F\,e^{-\rho x}} \to 0 \ (x \to \infty)$

$V(x)$ - par $\Rightarrow$ $\psi(x)$ - paridade definida





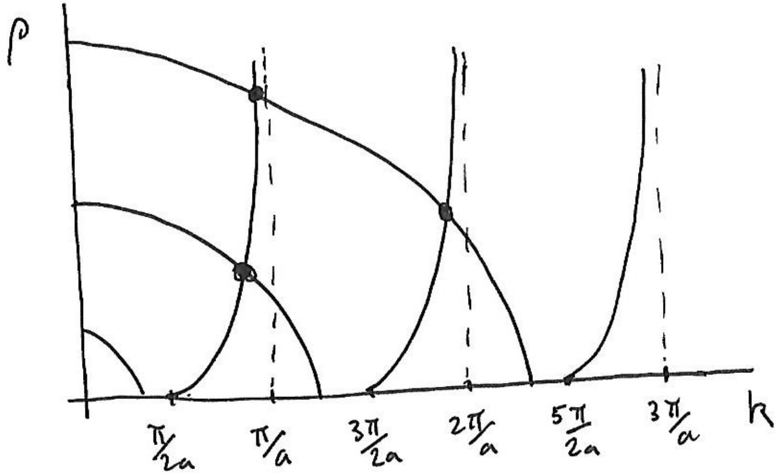
$$
\begin{cases}
\psi_{I} = \mp F e^{\rho x} & (x < -a) \\[2ex]
\psi_{II} = \underset{(\text{impar})}{C \operatorname{sen} kx} \quad \text{ou} \quad \underset{(\text{par})}{D \cos kx} & (-a < x < a) \\[2ex]
\psi_{III} = F e^{-\rho x}
\end{cases}
$$

<u>Solução ímpar</u>: $\psi_{II} = C \,\text{sen}\, kx \qquad \psi_{III} = F e^{-\rho x}$

$$\boxed{\rho^2 + k^2 = \frac{2mV_0}{\hbar^2}}$$ (círculo de raio $\sqrt{2mV_0}/\hbar$)

Contornos
$$\begin{cases} \psi_{II}(a) = \psi_{III}(a) & \Longrightarrow C \,\text{sen}\, ka = F e^{-\rho a} \\ \psi'_{II}(a) = \psi'_{III}(a) & \Longrightarrow kC \cos ka = -\rho F e^{-\rho a} \end{cases}$$

$$\Longrightarrow \cot g\, ka = -\frac{\rho}{k} \Longrightarrow \boxed{\rho = -k \cot g\, ka} > 0$$



$$\frac{\sqrt{2mV_0}}{\hbar} < \frac{\pi}{2a} \Longleftrightarrow V_0 < \frac{\pi^2\hbar^2}{8ma^2}$$ (não há estado ligado ímpar)

$$\frac{\pi}{2a} \leq \frac{\sqrt{2mV_0}}{\hbar} < \frac{3\pi}{2a} \Longleftrightarrow \frac{\pi^2\hbar^2}{8ma^2} \leq V_0 < \frac{9\pi^2\hbar^2}{8ma^2}$$ (1 estado)

$$\frac{3\pi}{2a} \leq \frac{\sqrt{2mV_0}}{\hbar} < \frac{5\pi}{2a} \Longleftrightarrow \frac{9\pi^2\hbar^2}{8ma^2} \leq V_0 < \frac{25\pi^2\hbar^2}{8ma^2}$$ (2 estados)

normalização: $|\psi(x)|^2$ - par $\Longrightarrow \int_{-\infty}^{\infty} |\psi|^2 dx = 2\int_0^{\infty} |\psi|^2 dx = 1$

$$= 2\left[|C|^2 \underbrace{\int_0^a \underbrace{\text{sen}^2 kx}_{(1-\cos 2kx)/2}\, dx}_{\frac{1}{2}\left[x\Big|_0^a - \frac{1}{2k}\text{sen}\, 2kx\Big|_0^a \right]} + |F|^2 \underbrace{\int_a^{\infty} e^{-2\rho x} dx}_{\frac{-1}{2\rho} e^{-2\rho x}\Big|_a^{\infty} = \frac{1}{2\rho}} \right] = 1$$

$$\begin{cases} |C|^2\left(a-\frac{1}{2k}\operatorname{sen}2ka\right)+|F|^2\frac{1}{\rho}e^{-2\rho a}=1 \\ C\operatorname{sen}ka=Fe^{-\rho a} \Rightarrow |F|^2=|C|^2\operatorname{sen}^2ka\, e^{2\rho a} \end{cases} \Rightarrow |C|^2\left(a-\underbrace{\frac{\operatorname{sen}2ka}{2k}}_{\frac{\operatorname{sen}ka\cos ka}{k}}+\frac{\operatorname{sen}^2ka}{\rho}\right)=1$$

$$\rho=-k\cot g\, ka=-k\frac{\cos ka}{\operatorname{sen}ka} \Rightarrow |C|^2\left[a-\frac{1}{k}\underbrace{\left(\operatorname{sen}ka\cos ka+\frac{\operatorname{sen}^3ka}{\cos ka}\right)}_{\frac{\operatorname{sen}ka\,(\cos^2ka+\operatorname{sen}^2ka)}{\cos ka}=\operatorname{tg}ka}\right]=1$$

$$|C|^2\left(a-\frac{\operatorname{tg}ka}{k}\right)=|C|^2\left(a+\frac{1}{\rho}\right)=1$$

$$\boxed{C=\frac{1}{\sqrt{a+1/\rho}}} \Rightarrow \boxed{F=\frac{e^{\rho a}}{\sqrt{a+1/\rho}}\operatorname{sen}ka}$$

Sol. ímpar

$$\begin{cases} \psi_I=-\frac{e^{\rho a}\operatorname{sen}ka}{\sqrt{a+1/\rho}}e^{\rho x} & (x<-a) \\ \psi_{II}=\frac{1}{\sqrt{a+1/\rho}}\operatorname{sen}kx & (-a<x<a) \\ \psi_{III}=\frac{e^{\rho a}\operatorname{sen}ka}{\sqrt{a+1/\rho}}e^{-\rho x} & (x>a) \end{cases}$$

Estados não ligados : $E > 0$ $\longrightarrow$ (incidencia)

incidente, reflectida

$$\begin{cases} \psi_I = A e^{ik_0 x} + B e^{-ik_0 x} \\ \psi_{II} = C \operatorname{sen} kx + D \cos kx \\ \psi_{III} = F e^{ik_0 x} \end{cases}$$

transmitida

$$k_0 = \sqrt{2mE}/\hbar$$

$$k = \sqrt{2m(E+V_0)}/\hbar$$

contorno em $x = a$

$$\begin{cases} C \operatorname{sen} ka + D \cos ka = F e^{ik_0 a} \\ k(C \cos ka - D \operatorname{sen} ka) = ik_0 F e^{ik_0 a} \end{cases}$$

contorno em $x = -a$

$$\begin{cases} -C \operatorname{sen} ka + D \cos ka = A e^{-ik_0 a} + B e^{ik_0 a} \\ k(C \cos ka + D \operatorname{sen} ka) = ik_0 (A e^{-ik_0 a} + B e^{ik_0 a}) \end{cases}$$

$\Downarrow$

$$\begin{cases} C \operatorname{sen}^2 ka + D \operatorname{sen} ka \cos ka = F e^{ik_0 a} \operatorname{sen} ka \\ C \cos^2 ka - D \operatorname{sen} ka \cos ka = i\frac{k_0}{k} F e^{ik_0 a} \cos ka \end{cases}$$

$$C = F e^{ik_0 a} \left(\operatorname{sen} ka + i\frac{k_0}{k} \cos ka \right)$$

$$\begin{cases} C \operatorname{sen} ka = F e^{ik_0 a} \left(\operatorname{sen}^2 ka + i\frac{k_0}{k} \operatorname{sen} ka \cos ka \right) \\ C \cos ka = F e^{ik_0 a} \left(\operatorname{sen} ka \cos ka + i\frac{k_0}{k} \cos^2 ka \right) \end{cases}$$

$$\begin{cases} C \operatorname{sen} ka \cos ka + D \cos^2 ka = F e^{ik_0 a} \cos ka \\ C \operatorname{sen} ka \cos ka - D \operatorname{sen}^2 ka = i\frac{k_0}{k} F e^{ik_0 a} \operatorname{sen} ka \end{cases}$$

$$D = F e^{ik_0 a} \left(\cos ka - i\frac{k_0}{k} \operatorname{sen} ka \right)$$

$$\begin{cases} D \cos ka = F e^{ik_0 a} \left(\cos^2 ka - i\frac{k_0}{k} \operatorname{sen} ka \cos ka \right) \\ D \operatorname{sen} ka = F e^{ik_0 a} \left(\operatorname{sen} ka \cos ka - i\frac{k_0}{k} \operatorname{sen}^2 ka \right) \end{cases}$$

do contorno em $x = -a$ $\Rightarrow$

$$\begin{cases} A e^{-ik_0 a} + B e^{ik_0 a} = F e^{ik_0 a}\left[\underbrace{(\cos^2 ka - \sin^2 ka)}_{\cos 2ka} - i\frac{k_0}{k}\underbrace{2\sin ka \cos ka}_{\sin 2ka}\right] \\ A e^{-ik_0 a} + B e^{ik_0 a} = -i\frac{k}{k_0} F e^{ik_0 a}\left[\underbrace{2\sin ka\cos ka}_{\sin 2ka} + i\frac{k_0}{k}\underbrace{(\cos^2 ka - \sin^2 ka)}_{\cos 2ka}\right] \\ \qquad = F e^{ik_0 a}\left(\cos 2ka - i\frac{k}{k_0}\sin 2ka\right) \end{cases}$$

$$\frac{2A e^{-2ik_0 a}}{F} = 2\cos 2ka - i\underbrace{\left(\frac{k}{k_0} + \frac{k_0}{k}\right)}_{(k^2+k_0^2)/k_0 k}\sin 2ka$$

$$\frac{A e^{-2ik_0 a}}{F} = \cos 2ka - i\left(\frac{k^2+k_0^2}{2k_0 k}\right)\sin 2ka$$

$$\left|\frac{F}{A}\right|^2 = T^{-1} = \underbrace{\cos^2 2ka}_{1-\sin^2 2ka} + \frac{(k^2+k_0^2)^2}{4k_0^2k^2}\sin^2 2ka = 1 + \underbrace{\left[\frac{(k^2+k_0^2)^2}{4k_0^2k^2} - 1\right]}\sin^2 2ka$$

$$\frac{k^4 + \overbrace{2k^2k_0^2 + k_0^4 - 4k_0^2k^2}^{-2k_0^2k^2}}{4k_0^2k^2} = \frac{(k^2-k_0^2)^2}{4k_0^2k^2}$$

$$\frac{(k^2-k_0^2)^2}{4k_0^2k^2} = \frac{V_0^2}{4E(E+V_0)}$$

$$\boxed{T^{-1} = 1 + \frac{V_0^2}{4E(E+V_0)} \operatorname{sen}^2 \frac{2a}{\hbar}\sqrt{2m(E+V_0)}}$$

$T = 1$ se $\frac{2a}{\hbar}\sqrt{2m(E+V_0)} = n\pi \quad (n = 1, 2, \ldots)$

$$\Downarrow$$

$$\boxed{E_n = \frac{n^2\pi^2\hbar^2}{8ma^2} - V_0}$$