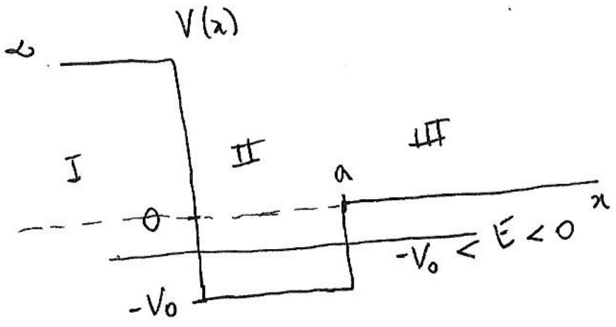
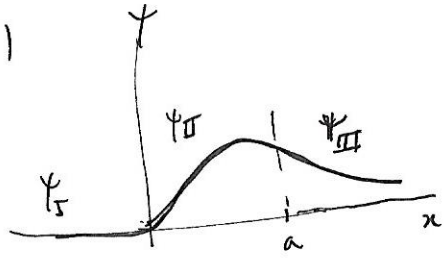
Estados ligados



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



$$\begin{cases} \text{região I}: \ \psi_I = 0 \\ \text{região II}: \ \dfrac{d^2\psi_{II}}{dx^2} + \overbrace{\dfrac{2m}{\hbar^2}\left(V_0 - |E|\right)}^{k_0^2}\psi_{II} = 0 \implies \psi_{II} = A e^{ik_0x} + B e^{-ik_0x} \quad (k_0 > 0) \\ \text{região III}: \ \dfrac{d^2\psi_{III}}{dx^2} - \underbrace{\dfrac{2m|E|}{\hbar^2}}_{\alpha^2}\psi_{III} = 0 \implies \psi_{III} = C e^{-\alpha x} \quad (\alpha > 0) \end{cases}$$

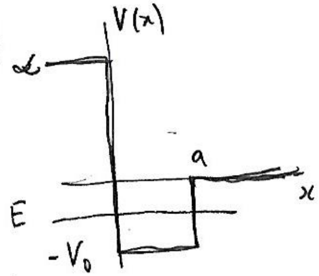
$$\boxed{\alpha^2 + k_0^2 = \frac{2mV_0}{\hbar^2} = v^2}$$

Condições de contorno

$$\begin{cases} \psi_I(0) = 0 = \psi_{II}(0) = A + B \implies B = -A \implies \psi_{II} = A\left(e^{ik_0x} - e^{-ik_0x}\right) = 2iA \operatorname{sen} k_0x \\ \psi_{II}(a) = \psi_{III}(a) \implies 2iA \operatorname{sen} k_0a = Ce^{-\alpha a} \\ \psi_{II}'(a) = \psi_{III}'(a) \implies k_0 2iA \cos k_0a = -\alpha Ce^{-\alpha a} \end{cases} \implies \operatorname{tg} k_0a = -\frac{k_0}{\alpha} \implies \boxed{\alpha = -k_0 \operatorname{cotg} k_0a}$$

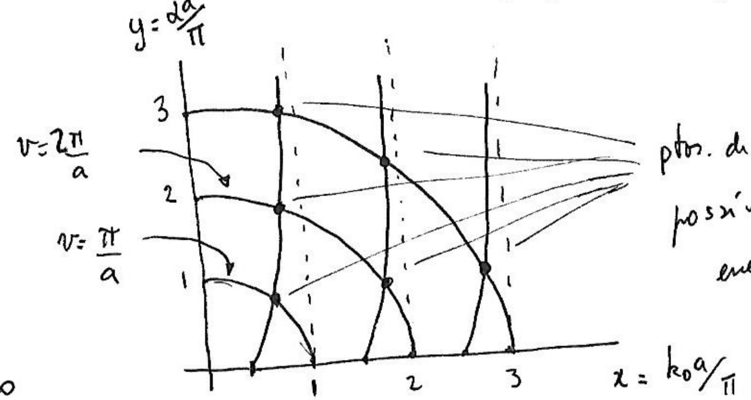
$$\begin{cases} \alpha^2 + k_0^2 = v^2 \\ \alpha = -k_0 \operatorname{cotg} k_0 a \end{cases}$$

$$v^2 = \frac{2mV_0}{\hbar^2} \qquad \alpha^2 = \frac{2m|E|}{\hbar^2} \qquad (E<0)$$



$$v = \pi/a \Rightarrow \begin{cases} \underbrace{\left(\frac{\alpha a}{\pi}\right)^2}_{y^2} + \underbrace{\left(\frac{k_0 a}{\pi}\right)^2}_{x^2} = 1 \\ \underbrace{\left(\frac{\alpha a}{\pi}\right)}_{y} = -\underbrace{\left(\frac{k_0 a}{\pi}\right)}_{x} \operatorname{cotg} \pi \underbrace{\left(\frac{k_0 a}{\pi}\right)}_{x} \end{cases}$$

$k_0 a$	$\operatorname{cotg} k_0 a$	$-k_0 \operatorname{cotg} k_0 a$
$\pi/2$	0	0
π	$-\infty$	∞
$3\pi/2$	0	0
2π	$-\infty$	∞



ptos. de interseção representam possíveis estados ligados, cujas energias são dadas por

$$E = -\frac{\hbar^2 \alpha^2}{2m}$$

$$v = \frac{\pi}{2a} \Rightarrow \frac{\pi^2}{4a^2} = \frac{2mV_0^{min}}{\hbar^2}$$

$$\Downarrow$$

$$V_0^{min} = \frac{\pi^2 \hbar^2}{8ma^2}$$ (valor mínimo p/ confinar uma partícula)

$$v = \frac{\pi}{a} \quad \begin{cases} y^2 + x^2 = 1 \quad (y = \sqrt{1-x^2}) \\ y = -x \operatorname{cotg} \pi x \end{cases} \Rightarrow h(x) = \sqrt{1-x^2} + x \operatorname{cotg} \pi x$$

(determinação das raízes de $h(x)$)

$$\Downarrow$$

$$x_n \Rightarrow y_n = \sqrt{1-x_n^2} \Rightarrow \alpha_n^2 = \frac{\pi^2}{a^2} y_n^2 \Rightarrow E = -\frac{\pi^2 \hbar^2}{2ma^2} y_n^2$$

$$\Updownarrow$$

$$V_0 = \frac{\pi^2 \hbar^2}{2ma^2}$$

Método de Newton

x	h(x)	h'(x)
0,500000	0,866025404	-2,148146596
0,903150	-2,44682558	-36,90041698
0,836841	-0,939613517	-14,23626418
0,770840	-0,24198092	-7,921052086
0,740291	-0,024165459	-6,426030257
0,736530	-0,000286438	-6,274694548
0,736484	-4,10991E-08	-6,272894065

h(x) = (1-x^2)^1/2 + x cot(pi x)
h'(x) = -x/(1-x^2)^1/2 + cot (pi x) - (pi x) cosec (pi x)

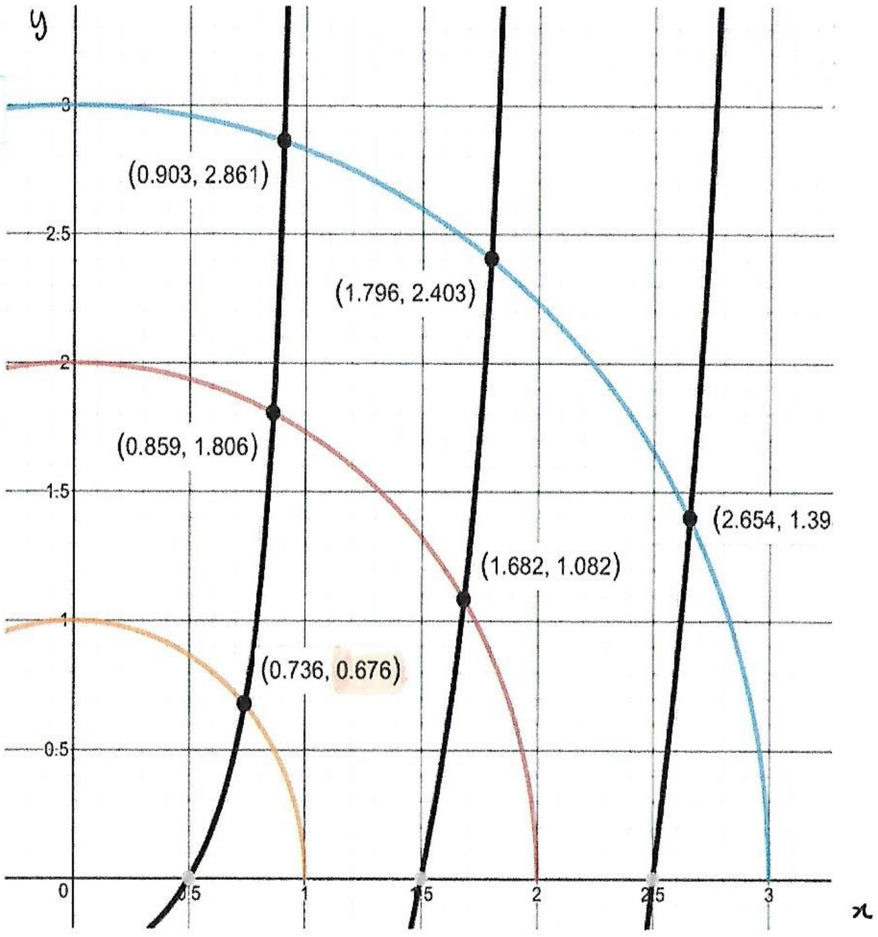
y=sqrt(1-x^2)   y=x*cot(pi x)
0,676454468

$\sqrt{1-x^2}$

$-x\cot(\pi x)$

$\sqrt{4-x^2}$

$\sqrt{9-x^2}$



$v = \frac{\pi}{a} \Rightarrow V_0 = \frac{\pi^2 \hbar^2}{2ma^2} \Rightarrow y = 0.676$

$E_1 = -\frac{\pi^2 \hbar^2}{2ma^2} (0.676)^2$

$\boxed{E_1 = -0.46\, V_0}$

energia do único estado ligado p/ $v = \pi/a$ (ou $V_0 = \frac{\pi^2\hbar^2}{2ma^2}$)

$\psi_I = 0 \qquad \psi_{II} = 2A \,\text{sen}\, k_0 x \qquad \psi_{III} = C e^{-\alpha x} \qquad \alpha = -k_0 \cot g\, k_0 a = \dfrac{-k_0}{tg k_0 a}$

normalização

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 4A^2 \int_0^a \underbrace{\text{sen}^2 k_0 x}_{(1-\cos 2k_0 x)/2}\, dx + C^2 \int_0^a e^{-2\alpha x} dx = 1$$

$$= 2A^2\left(a - \frac{1}{2k_0}\,\text{sen}\, 2k_0 a\right) + C^2 \frac{1}{2\alpha} e^{-2\alpha a} = 1$$

(contorno) $2A \,\text{sen}\, k_0 a = C e^{-\alpha a} \implies C^2 = 4A^2 \,\text{sen}^2 k_0 a\, e^{2\alpha a}$

$$\implies 2A^2\left(a - \frac{1}{2k_0}\,\overbrace{\text{sen}\, 2k_0 a}^{\text{sen}\, k_0 a \cos k_0 a / k_0}\right) + 2A^2 \frac{\text{sen}^2 k_0 a}{\alpha} = 1 \qquad \alpha = -k_0/tg k_0 a$$

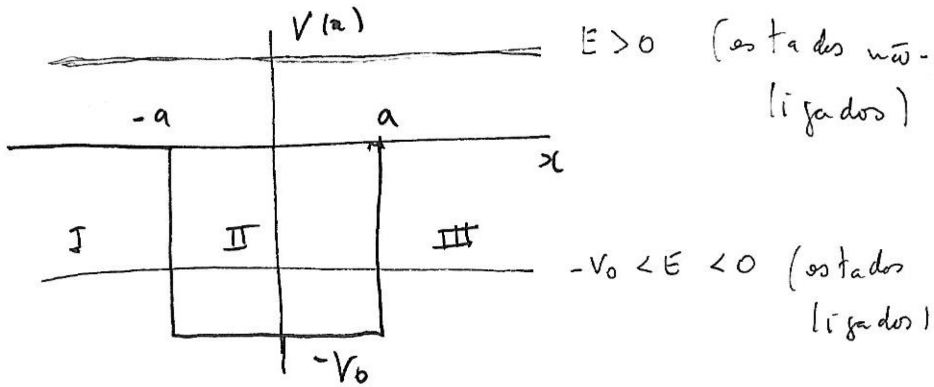
$$2A^2\left[a - \frac{1}{k_0}\underbrace{\left(\text{sen}\, k_0 a \cos k_0 a + \frac{\text{sen}^3 k_0 a}{\cos k_0 a}\right)}_{\frac{\text{sen}\, k_0 a\,(\cos^2 k_0 a + \text{sen}^2 k_0 a)}{\cos k_0 a} = tg\, k_0 a = -k_0/\alpha}\right] = 1 \implies 2A^2\left(a + 1/\alpha\right) = 1 \implies \boxed{A = \frac{1}{\sqrt{2(a+1/\alpha)}}}$$

$$\boxed{C = \sqrt{\frac{2}{(a+1/\alpha)}}\, e^{\alpha a}\, \text{sen}\, k_0 a}$$

$$\begin{cases} \psi_I = 0 & (x < 0) \\ \psi_{II} = \sqrt{\dfrac{2}{a+1/\alpha}}\,\text{sen}\, k_0 x & (0 < x < a) \\ \psi_{III} = \sqrt{\dfrac{2}{a+1/\alpha}}\, e^{\alpha a}\,\text{sen}\, k_0 a\, e^{-\alpha x} & (x > a) \end{cases}$$

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

$(V = 0)$

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

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

$(V = -V_0)$

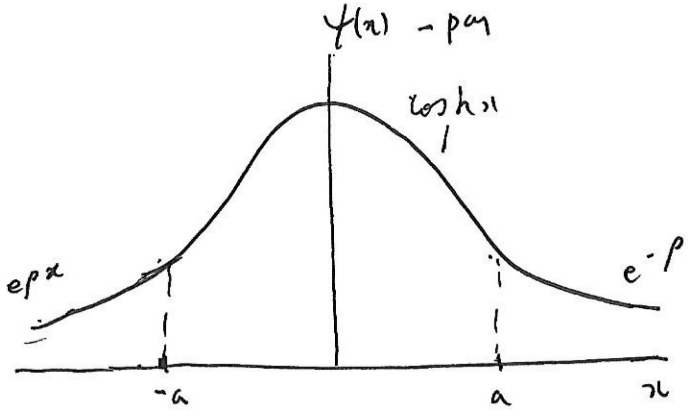
$$\boxed{\psi_{II} = C\sin kx + D\cos kx} \qquad k = \frac{\sqrt{2m(V_0 - |E|)}}{\hbar} \qquad \boxed{\rho^2 + k^2 = \frac{2mV_0}{\hbar^2}}$$

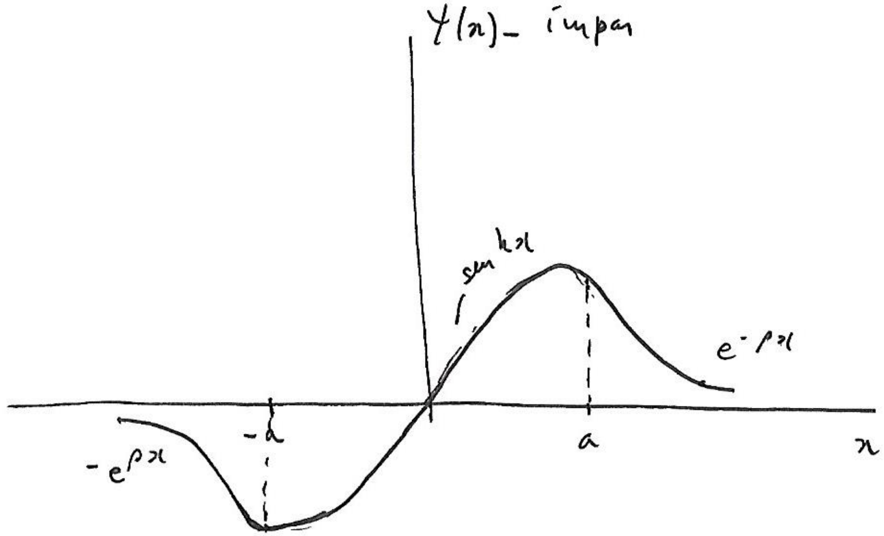
região III : $x > a$ $\Rightarrow$ $\frac{d^2\psi_{III}}{dx^2} = \rho^2\psi_{III}$

$(V = 0)$

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

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





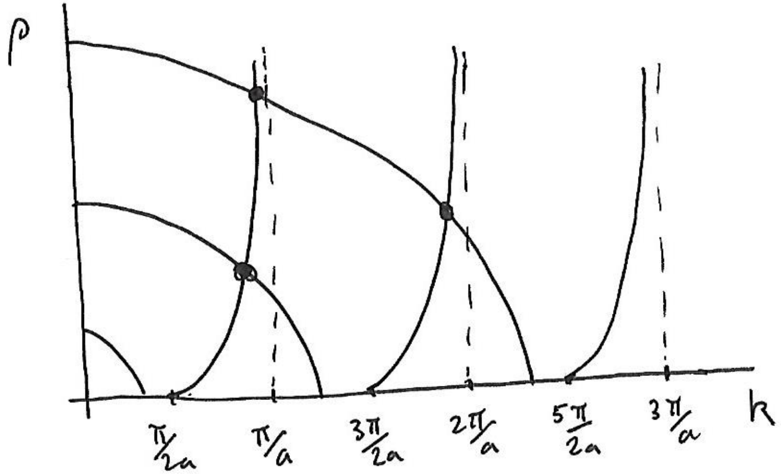
$$\begin{cases} \psi_{I} = \mp F e^{px} & (x < -a) \\ \psi_{II} = \underset{(\text{ímpar})}{C \operatorname{sen} kx} \quad \text{ou} \quad \underset{(\text{par})}{D \cos kx} & (-a < x < a) \\ \psi_{III} = F e^{-px} & \end{cases}$$

Solução ímpar: $\psi_{II} = C \operatorname{sen} kx$ $\qquad \psi_{III} = F e^{-\rho x}$

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

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

$$\implies \operatorname{cotg} ka = -\frac{\rho}{k} \implies \boxed{\rho = -k \operatorname{cotg} ka} > 0$$



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

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

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

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

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

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

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

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

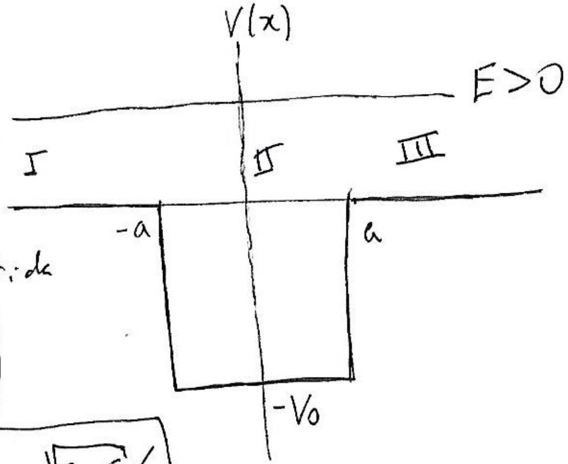
$$\boxed{C = \frac{1}{\sqrt{a + 1/\rho}}} \Rightarrow \boxed{F = \frac{e^{\rho a}}{\sqrt{a + 1/\rho}}\,\mathrm{sen}\,ka}$$

Sol. ímpar

$$\begin{cases} \psi_{I} = -\dfrac{e^{\rho a}\,\mathrm{sen}\,ka}{\sqrt{a + 1/\rho}}\, e^{\rho x} & (x < -a) \\[2ex] \psi_{II} = \dfrac{1}{\sqrt{a + 1/\rho}}\,\mathrm{sen}\,kx & (-a < x < a) \\[2ex] \psi_{III} = \dfrac{e^{\rho a}\,\mathrm{sen}\,ka}{\sqrt{a + 1/\rho}}\, e^{-\rho x} & (x > a) \end{cases}$$

Estados não ligados : $E>0$

$\xrightarrow{\text{incidência}}$



região I : $x < -a \Rightarrow -\dfrac{\hbar^2}{2m}\dfrac{d^2\psi_I}{dx^2} = E\psi_I$

$(V=0)$

$$\frac{d^2\psi_I}{dx^2} + \overbrace{\left(\frac{2m}{\hbar^2}E\right)}^{k_0^2}\psi_I = 0 \Rightarrow \boxed{\psi_I = \underbrace{Ae^{ik_0x}}_{\text{incidente}} + \underbrace{Be^{-ik_0x}}_{\text{refletida}}}$$

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

região II : $-a < x < a \Rightarrow -\dfrac{\hbar^2}{2m}\dfrac{d^2\psi_{II}}{dx^2} - V_0\psi_{II} = E\psi_{II}$

$(V=-V_0)$

$$\frac{d^2\psi_{II}}{dx^2} + \overbrace{\frac{2m}{\hbar^2}(E+V_0)}^{k^2}\psi_{II} = 0 \Rightarrow \boxed{\psi_{II} = C\,\mathrm{sen}\,kx + D\cos kx} \qquad k = \sqrt{2m(E+V_0)}/\hbar$$

região III : $x > a \Rightarrow -\dfrac{\hbar^2}{2m}\dfrac{d^2\psi_{III}}{dx^2} = E\psi_{III}$

$(V=0)$

$$\frac{d^2\psi_{III}}{dx^2} + \overbrace{\left(\frac{2mE}{\hbar^2}\right)}^{k_0^2}\psi_{III} = 0 \Rightarrow \boxed{\psi_{III} = \underbrace{Fe^{ik_0x}}_{\text{transmitida}}}$$

contorno
en $x=-a$ $\left\{\begin{array}{l}\psi_{I}(-a) = \psi_{II}(-a) \\ \psi'_{I}(-a) = \psi'_{II}(-a)\end{array}\right. \Longrightarrow \left\{\begin{array}{l} A e^{-ik_0a} + B e^{ik_0a} = -C \,\mathrm{sen}\,ka + D\cos ka \\ ik_0\left(A e^{-ik_0a} - B e^{ik_0a}\right) = k\left(C\cos ka + D\,\mathrm{sen}\,ka\right)\end{array}\right.$

$$C = F e^{ik_0a}\left(\mathrm{sen}\,ka + i\frac{k_0}{k}\cos ka\right) \Longrightarrow \left\{\begin{array}{l} C\,\mathrm{sen}\,ka = F e^{ik_0a}\left(\mathrm{sen}^2 ka + i\frac{k_0}{k}\mathrm{sen}\,ka\cos ka\right) \\ C\cos ka = F e^{ik_0a}\left(\mathrm{sen}\,ka\cos ka + i\frac{k_0}{k}\cos^2 ka\right)\end{array}\right.$$

$$D = F e^{ik_0a}\left(\cos ka - i\frac{k_0}{k}\mathrm{sen}\,ka\right) \Longrightarrow \left\{\begin{array}{l} D\cos ka = F e^{ik_0a}\left(\cos^2 ka - i\frac{k_0}{k}\mathrm{sen}\,ka\cos ka\right) \\ D\,\mathrm{sen}\,ka = F e^{ik_0a}\left(\mathrm{sen}\,ka\cos ka - i\frac{k_0}{k}\mathrm{sen}^2 ka\right)\end{array}\right.$$

$$\left\{\begin{array}{l} A e^{-ik_0a} + B e^{ik_0a} = F e^{ik_0a}\left[\underbrace{(\cos^2 ka - \mathrm{sen}^2 ka)}_{\cos 2ka} - i\frac{k_0}{k}\underbrace{2\,\mathrm{sen}\,ka\cos ka}_{\mathrm{sen}\,2ka}\right] \\ A e^{-ik_0a} - B e^{ik_0a} = \frac{-ik}{k_0} F e^{ik_0a}\left[\underbrace{2\,\mathrm{sen}\,ka\cos ka}_{\mathrm{sen}\,2ka} + i\frac{k_0}{k}\underbrace{(\cos^2 ka - \mathrm{sen}^2 ka)}_{\cos 2ka}\right] \\ \qquad = F e^{ik_0a}\left(\cos 2ka - i\frac{k}{k_0}\mathrm{sen}\,2ka\right)\end{array}\right.$$

$$2A e^{-ik_0a} = F e^{ik_0a}\left[2\cos 2ka - i\left(\frac{k}{k_0} + \frac{k_0}{k}\right)\mathrm{sen}\,2ka\right]$$

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

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

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

contorno em $x = a$ $\begin{cases} \psi_{II}(a) = \psi_{III}(a) \\ \psi'_{II}(a) = \psi'_{III}(a) \end{cases} \Rightarrow \begin{cases} C \,\text{sen}\, ka + D \cos ka = F e^{ik_0 a} \\ k(C \cos ka - D \,\text{sen}\, ka) = i k_0 F e^{ik_0 a} \end{cases}$

$\begin{pmatrix} \text{sen}\, ka \\ \cos ka \end{pmatrix}$ $\begin{pmatrix} \cos ka \\ \text{sen}\, ka \end{pmatrix}$

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

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

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

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

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

coeficiente de transmissão

$$T = \left|\frac{F}{A}\right|^2$$

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

$$\begin{cases} \frac{(k^2+k_0^2)^2}{4k_0^2k^2} - 1 = \frac{k^4 + \overbrace{2k^2k_0^2 + k_0^4 - 4k_0^2k^2}^{-2k_0^2k^2}}{4k_0^2k^2} = \frac{(k^2-k_0^2)^2}{4k_0^2k^2} \\ \frac{(k^2-k_0^2)^2}{4k_0^2k^2} = \frac{V_0^2}{4E(E+V_0)} \end{cases}$$

$$\begin{cases} k_0 = \sqrt{2mE}/\hbar \Rightarrow k_0^2 = 2mE/\hbar^2 \\ k = \sqrt{2m(E+V_0)}/\hbar \Rightarrow k^2 = 2m(E+V_0)/\hbar^2 \end{cases}$$

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

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

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

$$\Downarrow$$

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