Equation de Schrödinger indépendante du temps en représentation x   d=1

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

V(x) = 0

$$-\frac{d^2}{dx^2}\psi = \frac{2mE}{\hbar^2}\psi \qquad \psi = N e^{\pm i\sqrt{\frac{2mE}{\hbar^2}}x}$$

$$\psi_E(x) = N e^{ikx} \qquad k = \pm\frac{\sqrt{2mE}}{\hbar} \qquad E_k = \frac{\hbar^2 k^2}{2m}$$

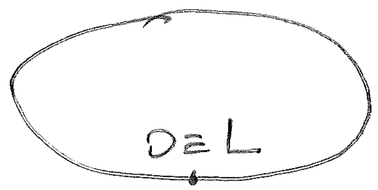
solution générale $\boxed{\psi_k(x) = A e^{ikx} + B e^{-ikx}}$

$$\boxed{\psi} \sim \frac{1}{\sqrt{\ell}}$$

$$\begin{cases} \psi_k(x) = \dfrac{1}{\sqrt{2\pi}} e^{ikx} \\ \phi_p(x) = \dfrac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar}px} \end{cases}$$

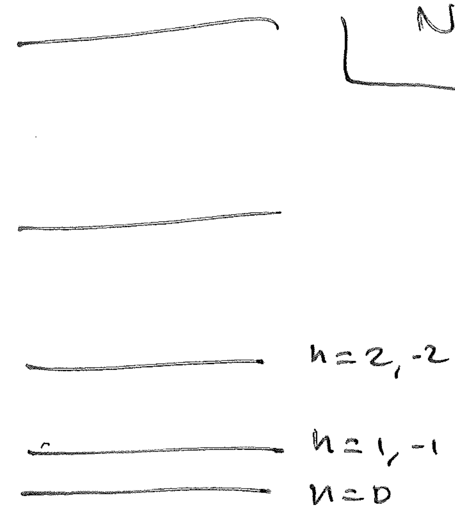
Normalisée à la δ

Conditions aux limites périodiques

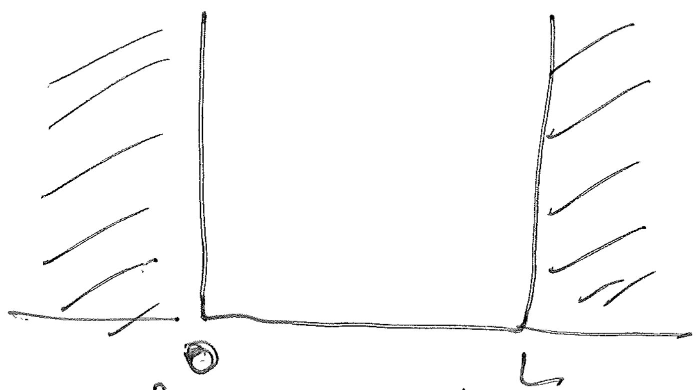


$$\psi_n(x) = \frac{e^{ik_n x}}{\sqrt{L}} \qquad \boxed{k_n = \frac{2\pi}{L} n} \qquad n \in \mathbb{Z}$$

$$E_n = \frac{\hbar^2}{2m}\left(\frac{2\pi}{L} n\right)^2$$



Condition aux limites ouvertes / libres



$$V(x) = \begin{cases} 0 & 0 < x < L \\ \infty & x < 0 \quad x > L \end{cases}$$

$$\psi(0) = \psi(L) = 0$$

$\psi(0) = 0 \qquad A + B = 0 \qquad A = -B$

$\psi_k(x) = 2iA \sin(kx)$

$\psi(L) = 0 \qquad \sin(kL) = 0 \longrightarrow \begin{cases} kL = n\pi \qquad n \in \mathbb{N}^* \qquad n = 1, 2, \ldots \\ \boxed{k_n = \frac{n\pi}{L}} \end{cases}$

(2)

$$\psi_n(x) = \underbrace{2iA}_{N} \sin\left(\frac{n\pi}{L}x\right) = 2iA\,\frac{e^{i\frac{n\pi}{L}x} - e^{-i\frac{n\pi}{L}x}}{2i}$$

$$N^{-1} = \left[\int_0^L dx \,\sin^2\left(\frac{n\pi}{L}x\right)\right]^{1/2} \qquad \frac{e^{i\frac{n\pi}{L}x}}{\sqrt{L}} \qquad \frac{e^{-i\frac{n\pi}{L}x}}{\sqrt{L}}$$

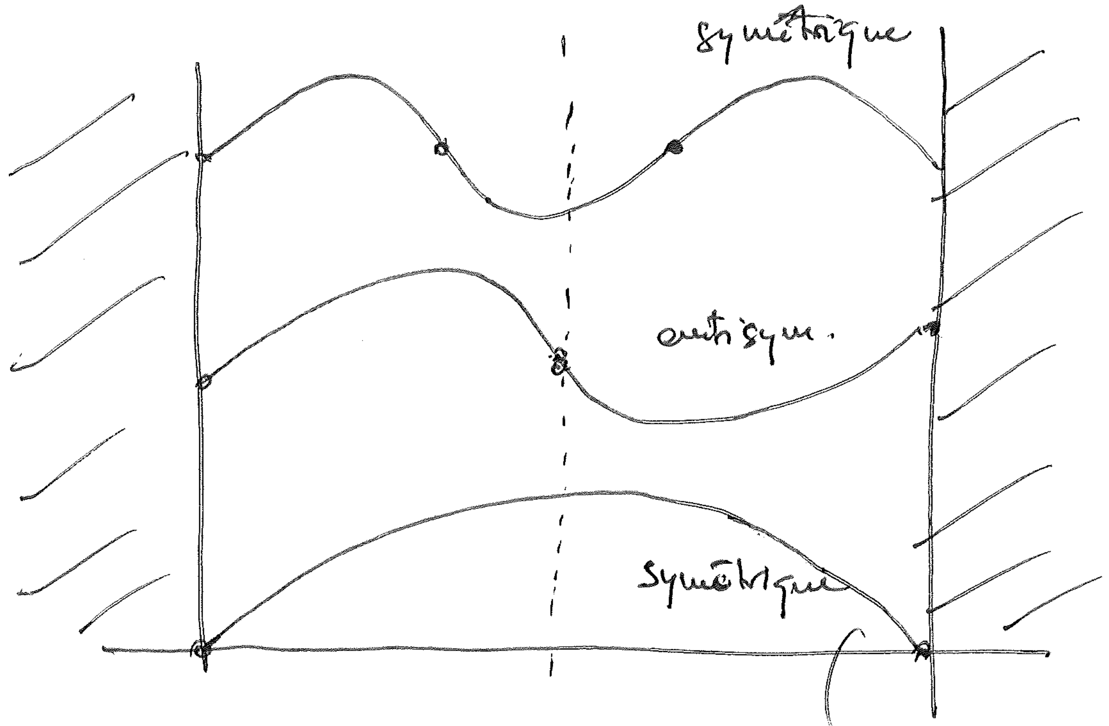
$$= \frac{1}{\sqrt{2}}\left[\frac{e^{i\frac{n\pi}{L}x}}{\sqrt{L}} - \frac{e^{-i\frac{n\pi}{L}x}}{\sqrt{L}}\right]$$

$$= 2i\,\frac{1}{\sqrt{2L}}\sin\left(\frac{n\pi}{L}x\right) = \cancel{i}\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right)$$

$$2A = \sqrt{\frac{2}{L}}$$

$$\boxed{\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right)}$$

$$E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2$$



$n=3$

$n=2 \quad \sqrt{\frac{2}{L}}\sin\left(\frac{2\pi}{L}x\right)$

$n=1 \quad \sqrt{\frac{2}{L}}\sin\left(\frac{\pi}{L}x\right)$

valeurs propres non dégénérées

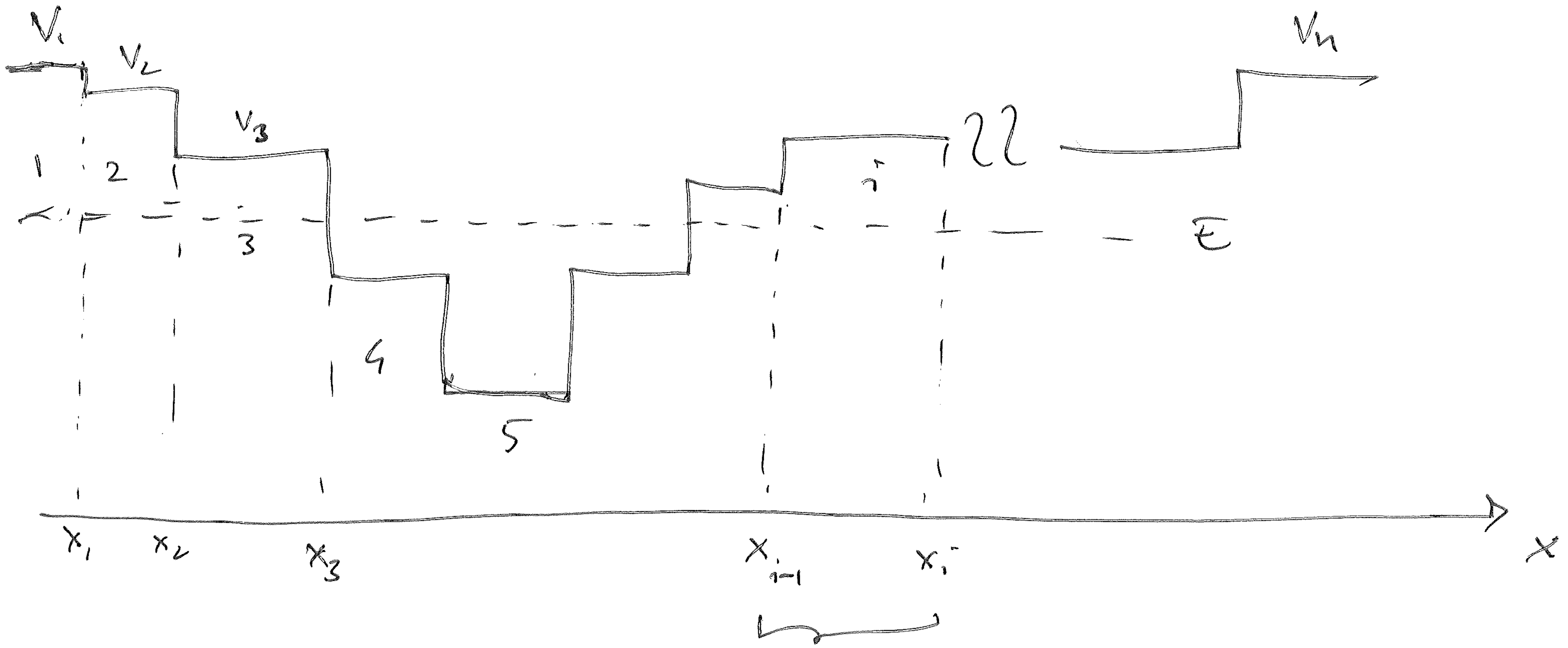
de noeuds = $n-1$

$$E_{n=1} = \frac{\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2 \neq 0$$

énergie de point zéro

$$\Delta x = L \qquad \Delta p \sim \frac{\hbar}{L} \qquad E = \frac{p^2}{2m} \approx \frac{(\Delta p)^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{1}{L}\right)^2$$

Solution générale de l'équation de Schrödinger pour un puit de potentiel constant par morceaux



$$V(x) = \begin{cases} V_1 & x \leq x_1 \\ V_2 & x_1 < x \leq x_2 \\ \vdots \end{cases}$$

n morceaux

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

n morceaux

2n variables A_i, B_i

$$\psi = A_i e^{ik_i x} + B_i e^{-ik_i x}$$

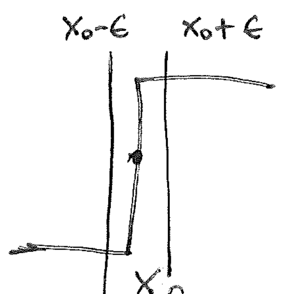
$$= A_i e^{-q_i x} + B_i e^{q_i x}$$

$$k_i = \begin{cases} \sqrt{\dfrac{2m(E - V_i)}{\hbar}} & E > V_i \\ i\,\dfrac{\sqrt{2m\,|E - V_i|}}{\hbar} = i q_i & E < V_i \end{cases}$$

Conditions de passage

: $n-1$ points de raccords

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



$$\int_{x_0-\epsilon}^{x_0+\epsilon} dx\,\frac{d^2\psi}{dx^2} = \psi'(x_0+\epsilon) - \psi'(x_0-\epsilon)$$

$$= \int_{x_0-\epsilon}^{x_0+\epsilon} dx\, -\frac{2m}{\hbar^2}[E - V(x)]\,\psi(x) \xrightarrow{\epsilon \to 0} 0$$

$\psi(x)$ normalisable $\int |\psi(x)|^2 < \infty$ (4)

$\psi(x) \sim \frac{1}{x^\alpha}$

deux conditions

$$\begin{cases} \psi'(x_0^-) = \psi'(x_0^+) \\ \psi(x_0^-) = \psi(x_0^+) \end{cases} \Leftarrow$$

$\psi'(x_0^-) = \psi'(x_0^+)$ dérivée première est continue

$\psi'(x_0)$ existe $\Rightarrow$ $\psi(x)$ est continue en x_0

$\psi(x_0^-) = \psi(x_0^+)$

$$\begin{cases} 2(n-1) = 2n-2 \\ 2n \end{cases}$$

$2(n-1) = 2n-2$ conditions de passage + 1 condition de normalisation (quand elle est applicable)

$2n$ variables

Cas spécifiques

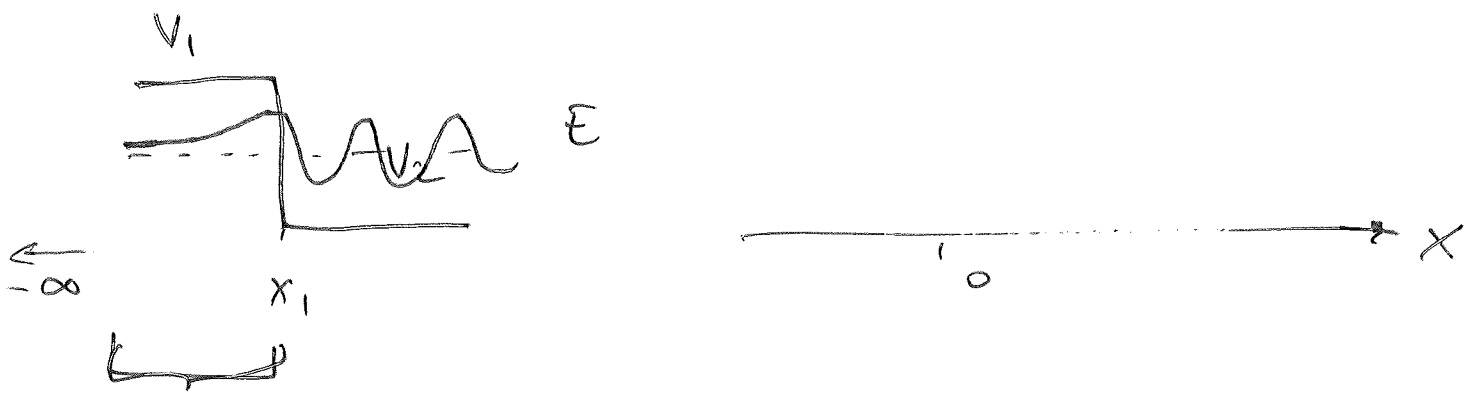
1) ETAT LIÉ : $E < V_1$, $E < V_n$

$\begin{cases} 2n-2 \text{ variables} \\ \text{pour } 2n-1 \text{ conditions} \end{cases}$

condition sur l'énergie E

$\Rightarrow$ spectre discret

spectre non dégénéré



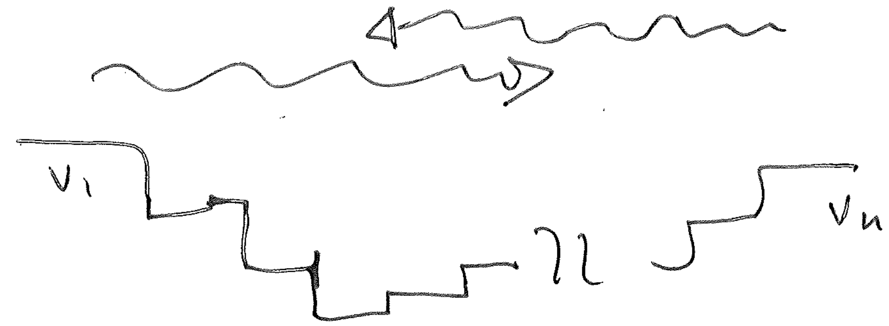
$\cancel{A_1 e^{-q_1 x}} + B_1 e^{q_1 x}$

2) État libre $E > V_1$, $E > V_n$

2n−2 conditions de passage
2n variables } 2 variables libres

$$\psi = A^{(+)}\psi^{(+)} + A^{(-)}\psi^{(-)}$$

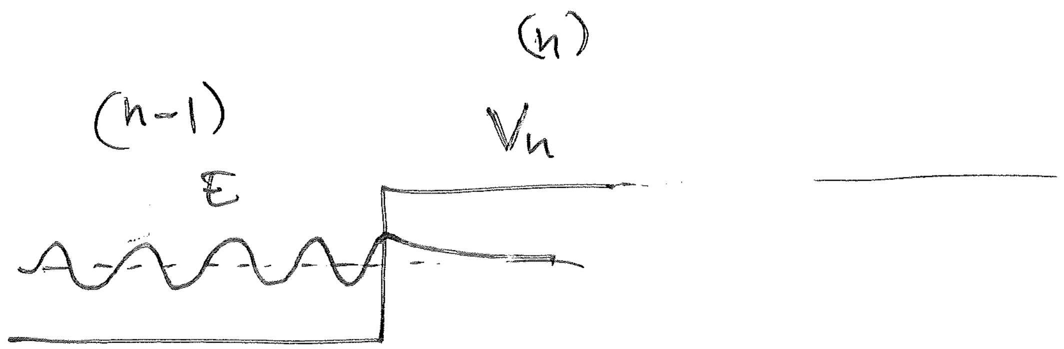
2 solutions dégénérées $\psi_E^{(\pm)}$



Avec les ψ_E $E > V_1, V_n$
on construit des paquets d'ondes pour avoir des états physique.

3) État semi-libre

$E > V_1$
$E < V_n$



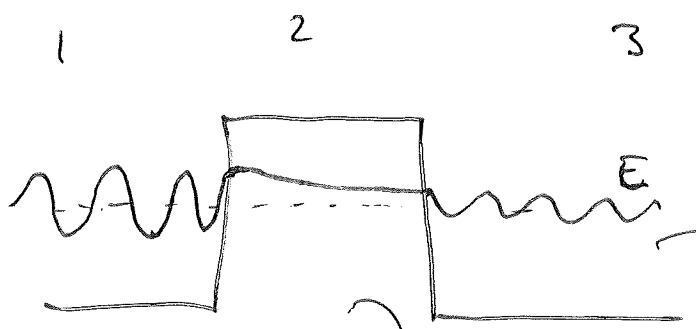
$A_{n-1} e^{ik_{n-1}x} + B_{n-1} e^{-ik_{n-1}x}$

$A_n e^{-\rho_n x}$
onde évanescente

2n−2 conditions
2n−1 variables

solution non normalisable

Exemple
barrière finie



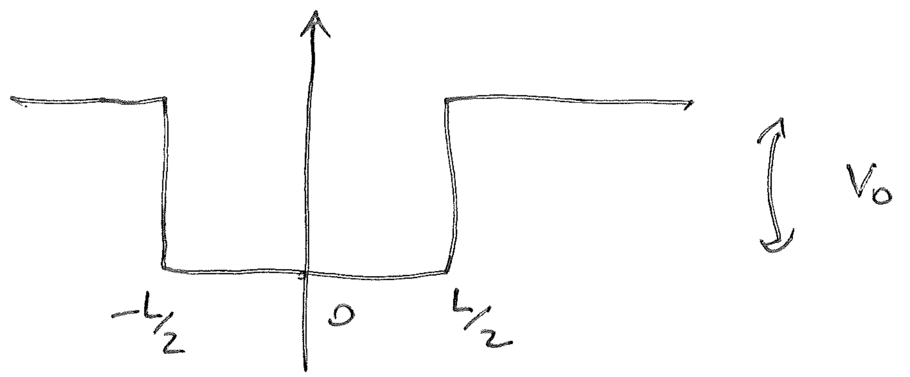
EFFET TUNNEL

$A_1 e^{ik_1x} + B_1 e^{-ik_1x}$

$A_2\, e^{-\rho_2 x} + B_2\, e^{\rho_2 x}$

$A_3\, e^{ik_3x} + B_3\, e^{-ik_3x}$

Puits de potentiel finie



① ② ③

Cherche des états liés

$E < V_0$

1) $A_1 e^{+\rho x}$

2) $A_2 e^{ik_\cdot x} + B_2 e^{-ik \cdot x}$

3) $A_3 \; e^{-\rho x}$

$\rho = \dfrac{\sqrt{2m|E-V_0|}}{\hbar}$

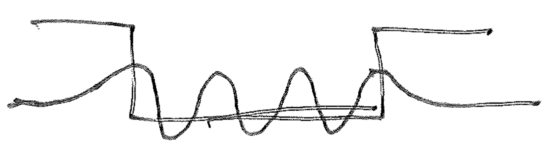
$k = \dfrac{\sqrt{2mE}}{\hbar}$

Symétrique

1) $A e^{\rho x}$

2) $B \cos(kx)$

3) $A e^{-\rho x}$

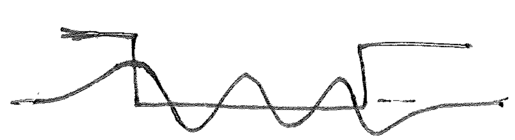


Anti-symétrique

1) $A' e^{\rho x}$

2) $B' \sin(kx)$

3) $-A' e^{-\rho x}$



$\langle \psi | \hat{P} | \phi \rangle = \int dx \cdot \psi^* P \phi = (\langle \phi | \hat{P} | \psi \rangle)^*$

symétrie par inversion

si $\psi(x)$ est solution $\Rightarrow$ $\psi(-x)$ est aussi solution

$\psi(x) = e^{i\phi} \cdot \psi(-x)$

$\hat{P} \psi(x) = \psi(-x)$ opérateur de parité

$\hat{P}$ opérateur hermitique

$\hat{P}\psi(x) = \psi(-x) = e^{i\phi} \psi(x)$

$e^{i\phi}$ valeur propre de $\hat{P} \rightarrow e^{i\phi} \in \mathbb{R}$

$\phi = 0, \pi$

$\psi(x) = \pm \psi(-x)$

$\psi(x)$ a une parité définie

Passage entre (1) et (2)

symétrique

$$\psi(-\tfrac{L}{2}^-) = \psi(-\tfrac{L}{2}^+)$$

$$A e^{-\rho \frac{L}{2}} = B \cos\left(k \tfrac{L}{2}\right)$$

$$\psi'(\quad) = \psi'(\quad)$$

$$A\rho\, e^{-\rho \frac{L}{2}} = B k \sin\left(k \tfrac{L}{2}\right)$$

$$\rho/k = \tan\left(\tfrac{kL}{2}\right)$$

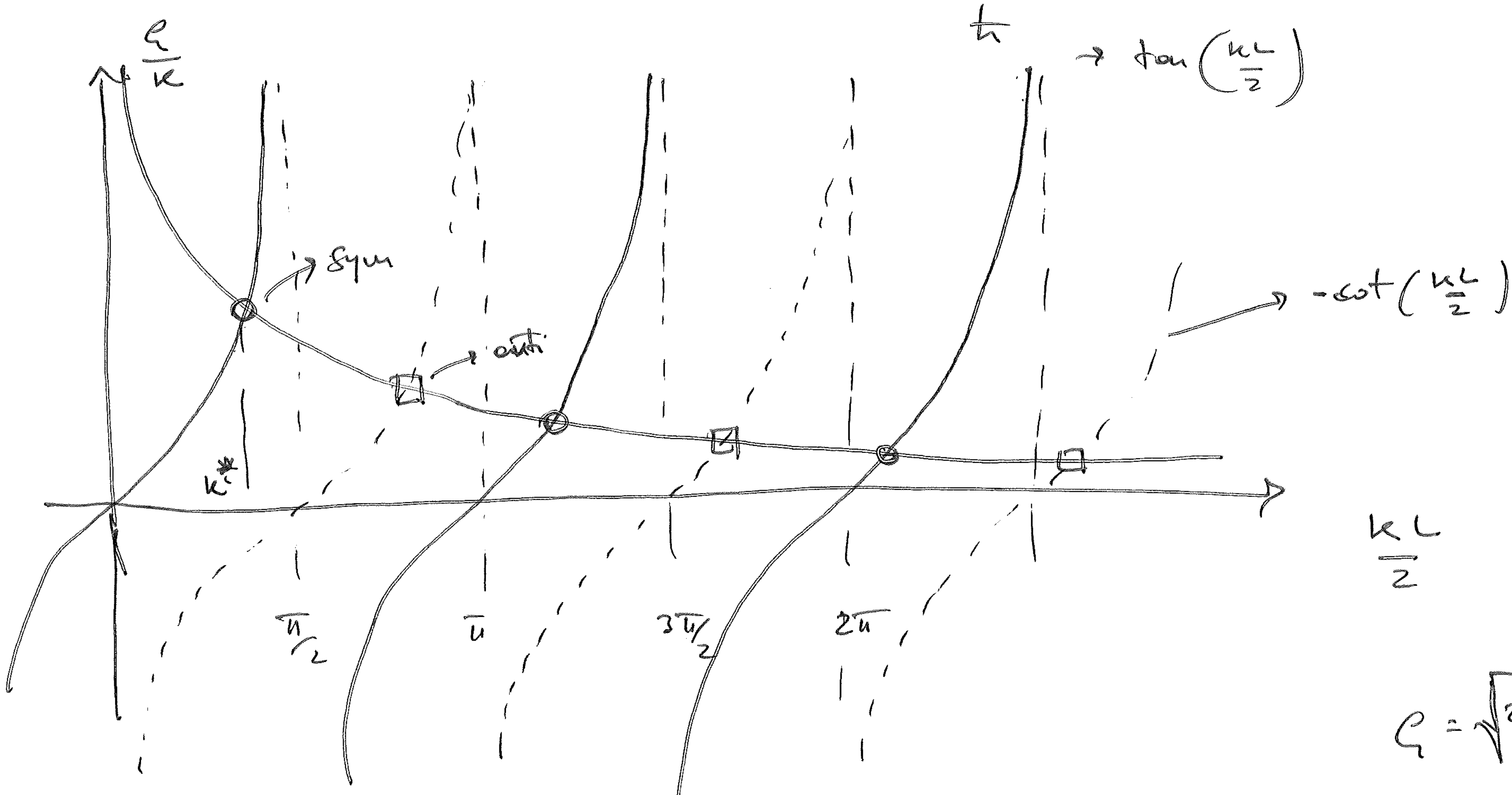
antisymétrique

$$A' e^{-\rho \frac{L}{2}} = -B' \sin\left(k \tfrac{L}{2}\right)$$

$$A'\rho\, e^{-\rho \frac{L}{2}} = B' k \cos\left(\tfrac{kL}{2}\right)$$

$$\rho/k = -\cot\left(\tfrac{kL}{2}\right)$$

condition sur $k \Rightarrow$ $k = \frac{\sqrt{2mE}}{\hbar}$



$E < V_0$

$$k \le k_{max} = \frac{\sqrt{2mV_0}}{\hbar}$$

∃ au moins un état lié ?

$$\frac{\rho}{k} = \tan\left(\tfrac{kL}{2}\right) \qquad k \le k_{max}$$

$$\rho = \sqrt{\frac{2m(V_0-E)}{\hbar^2}} = \sqrt{k_{max}^2 - k^2}$$

$$\rho/k = \sqrt{\frac{k_{max}^2}{k^2} - 1} = \tan\left(\tfrac{kL}{2}\right) \qquad \frac{k_{max}^2}{k^2} - 1 = \tan^2\left(\tfrac{kL}{2}\right)$$

8

$$\frac{k_{max}^2}{k^2} = \tan^2(kL) + 1$$

$$k_{max}^2 = (\underbrace{\tan^2(kL)+1}_{\geq 1}) k^2 \geq k^2 \qquad k_{max} \geq k$$

$\exists$ un état lié symétrique pour toute valeur de V_0.