

La science quantique

Une vision singulière

IV) Puits de potentiel

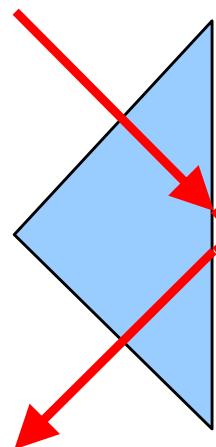
P.A. Besse

Réflexion et transmission

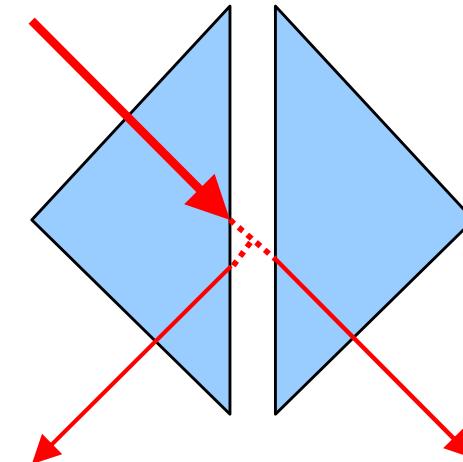
Effet tunnel

Comparaison: photons \leftrightarrow électrons

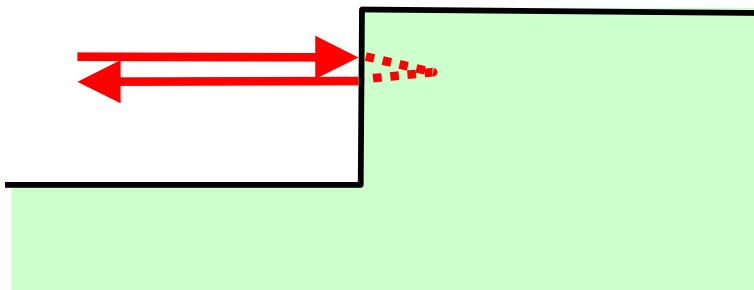
Réflexion totale



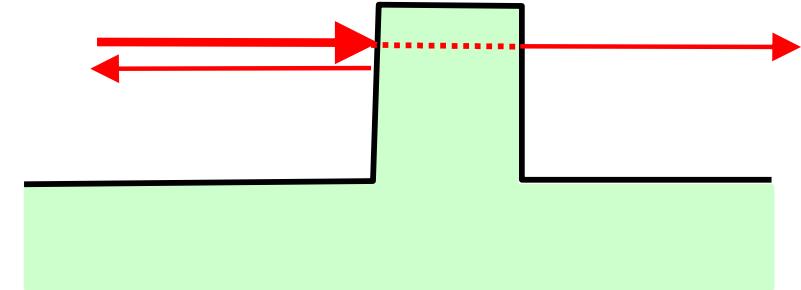
Réflexion frustrée

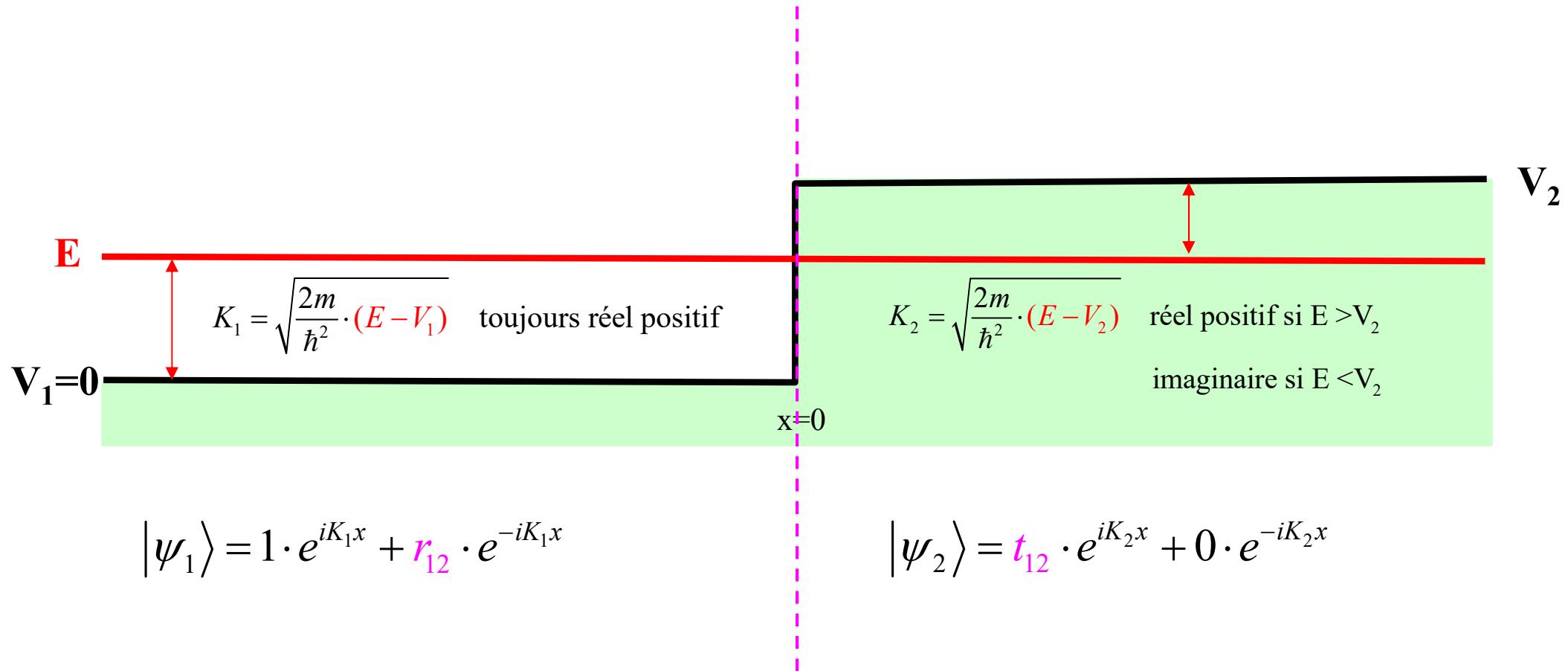


Step de potentiel



Effet tunnel

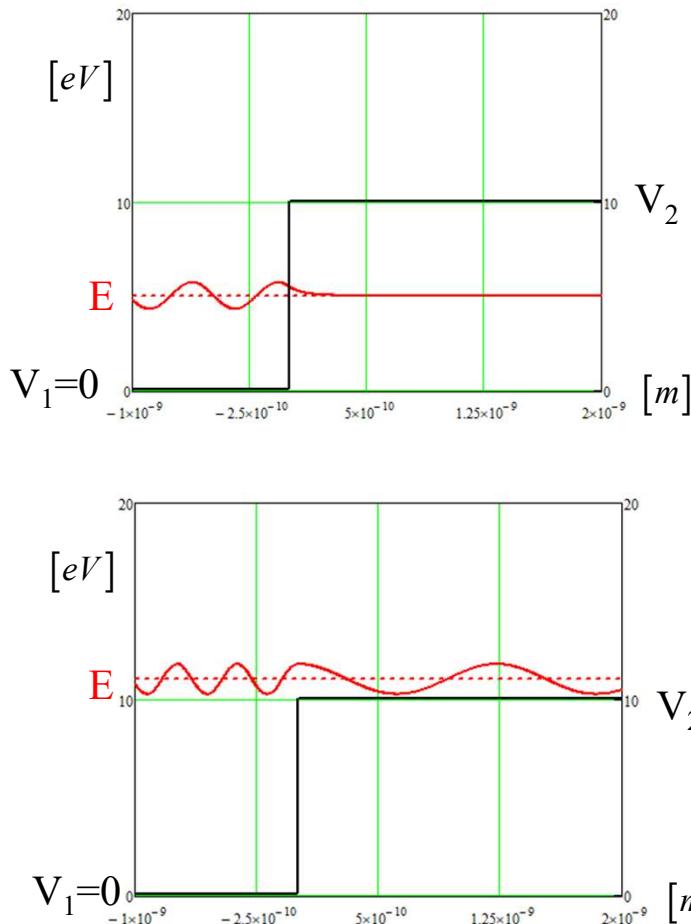




À l'interface, la fonction d'onde et sa dérivée sont continues* → déterminer r_{12} et t_{12}

* Voir Cohen-Tannoudji Livre I p. 66.

Réflexion sur un step de potentiel

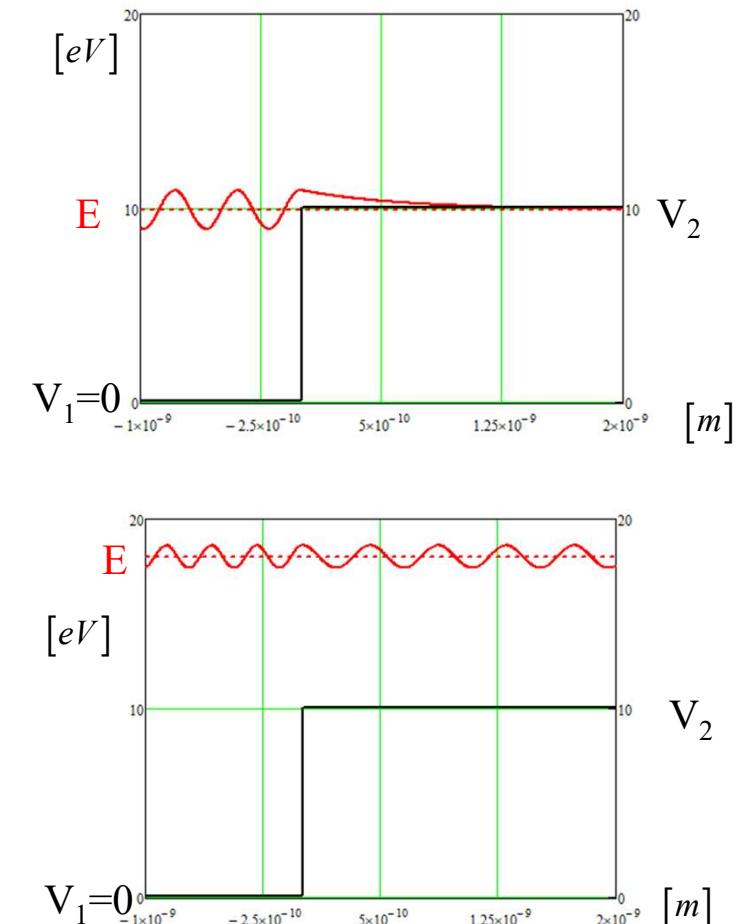


$$r_{12} = \frac{K_1 - K_2}{K_1 + K_2}$$

$$t_{12} = \frac{2K_1}{K_1 + K_2}$$

$$R = |r_{12}|^2$$

$$T = 1 - R = \frac{K_2}{K_1} \cdot |t_{12}|^2$$



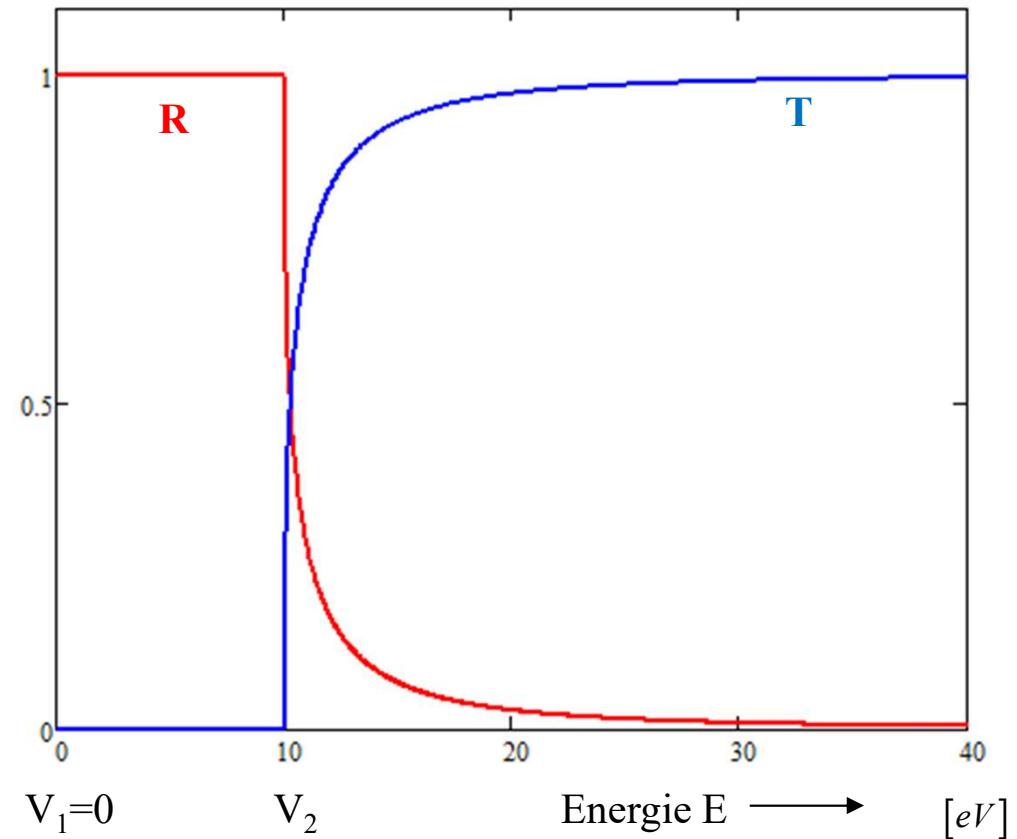
Réflexion sur un step de potentiel

$$r_{12} = \frac{K_1 - K_2}{K_1 + K_2}$$

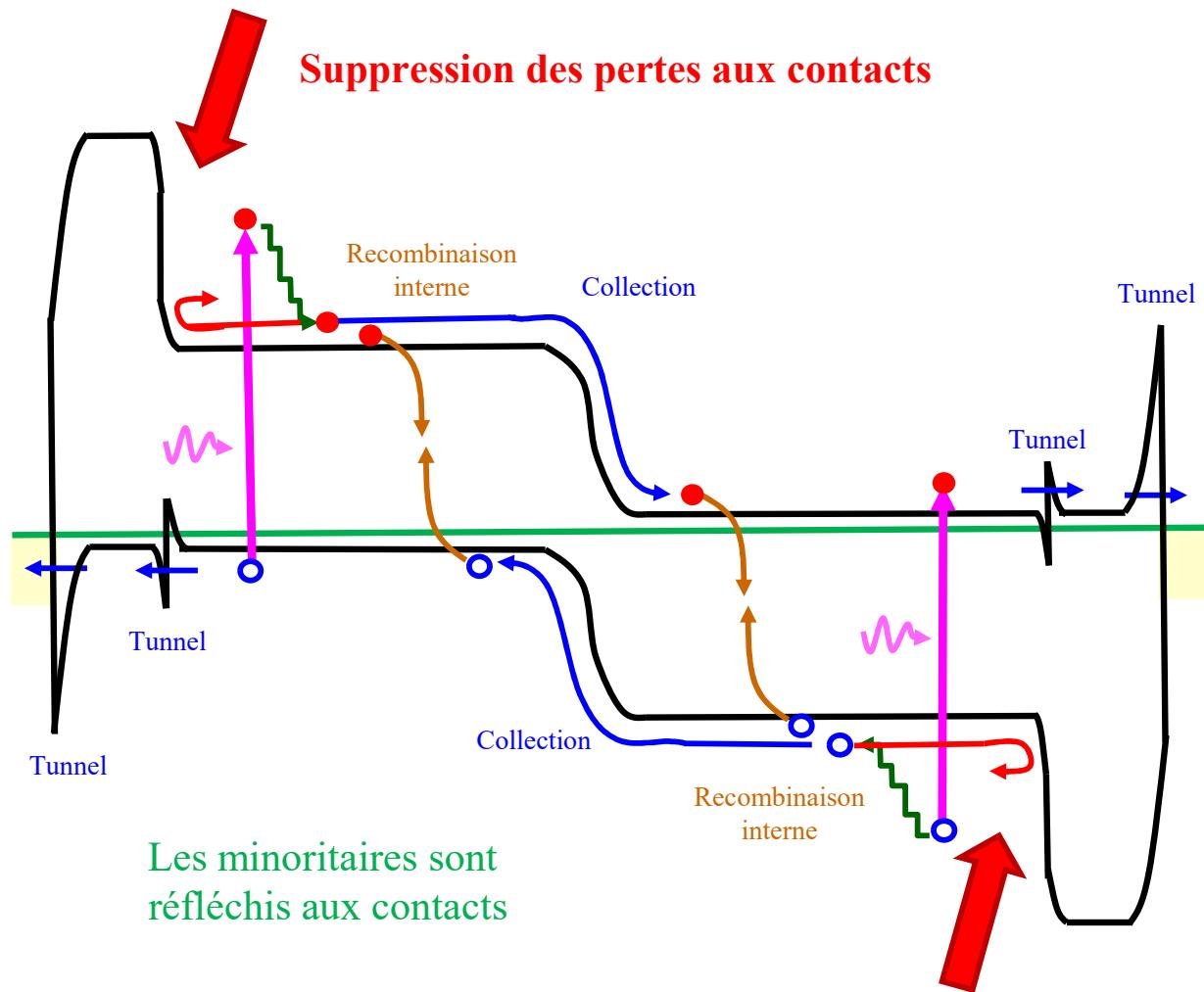
$$t_{12} = \frac{2K_1}{K_1 + K_2}$$

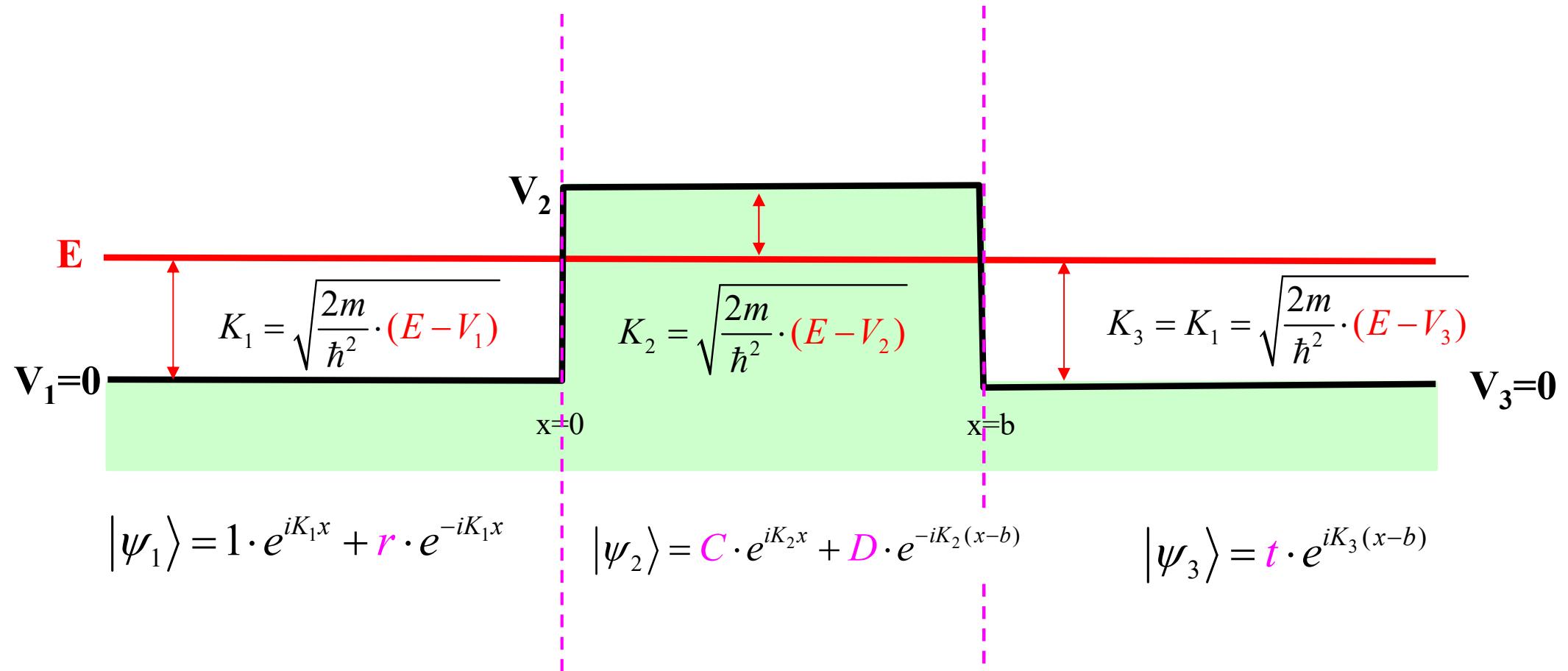
$$R = |r_{12}|^2$$

$$T = 1 - R$$



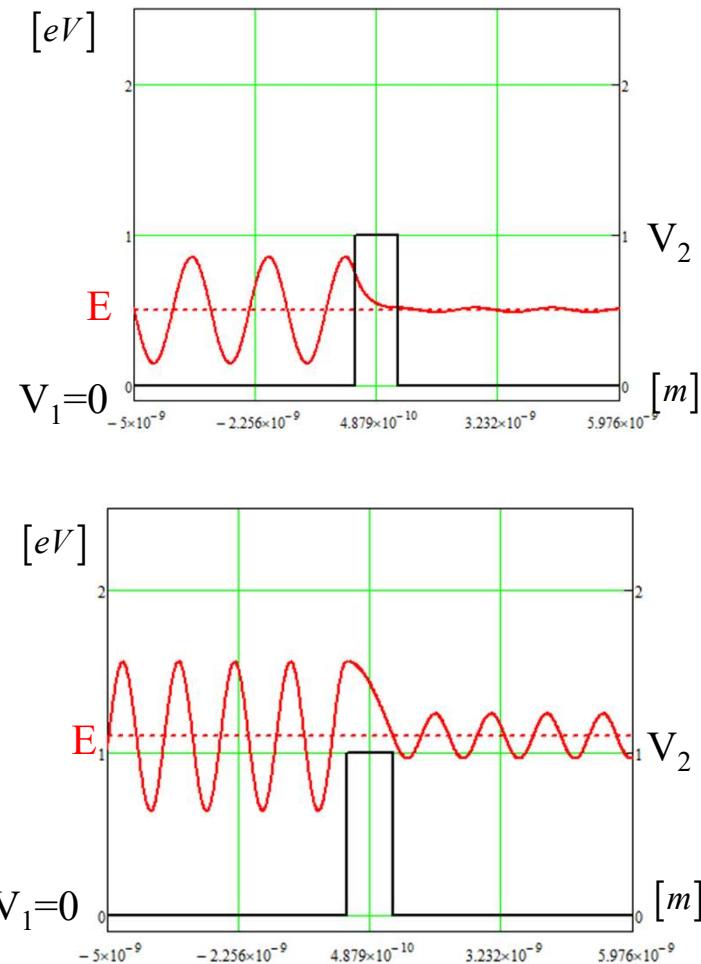
Réflexion: cellule solaire hétérostructure réflexive





Aux interfaces, la fonction d'onde et sa dérivée sont continues → déterminer r et t

Effet tunnel

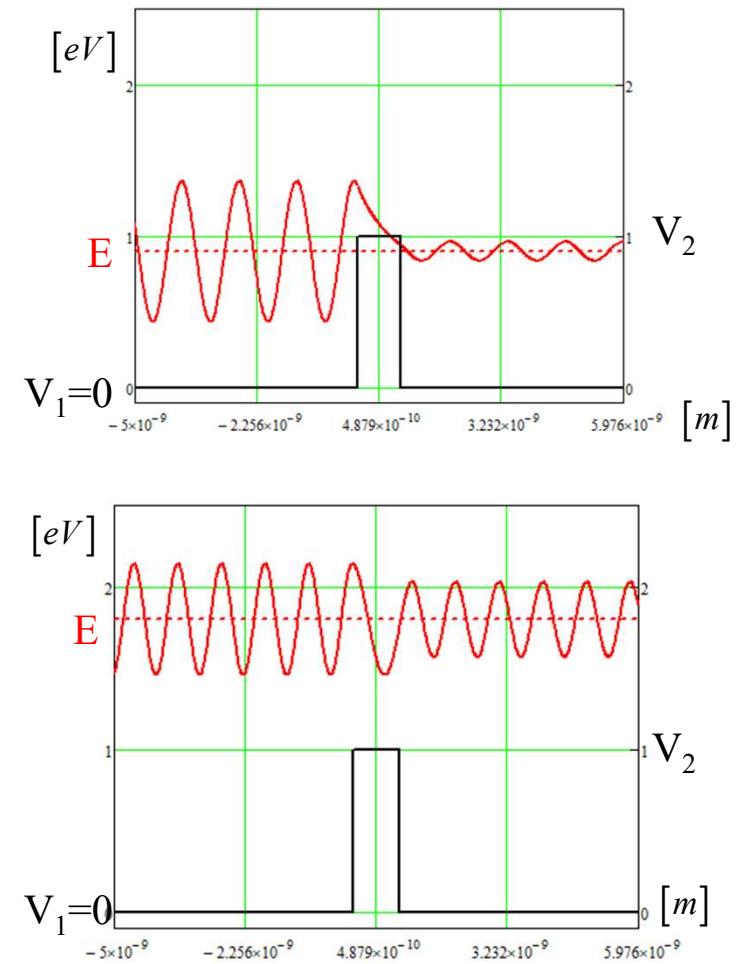


$$r_{12} = -r_{23} = \frac{K_1 - K_2}{K_1 + K_2}$$

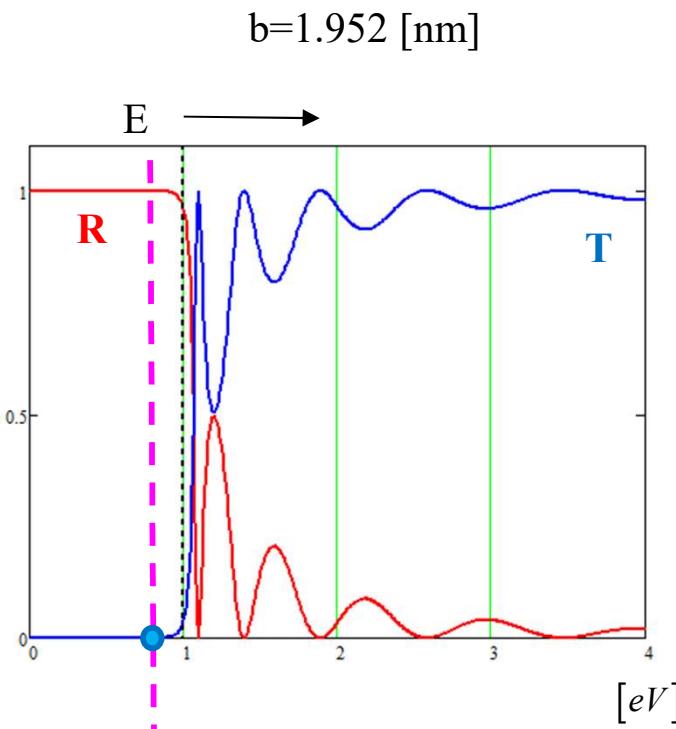
$$r = \frac{r_{12} + r_{23} \cdot e^{2iK_2 b}}{1 + r_{12} \cdot r_{23} \cdot e^{2iK_2 b}}$$

$$R = |r|^2$$

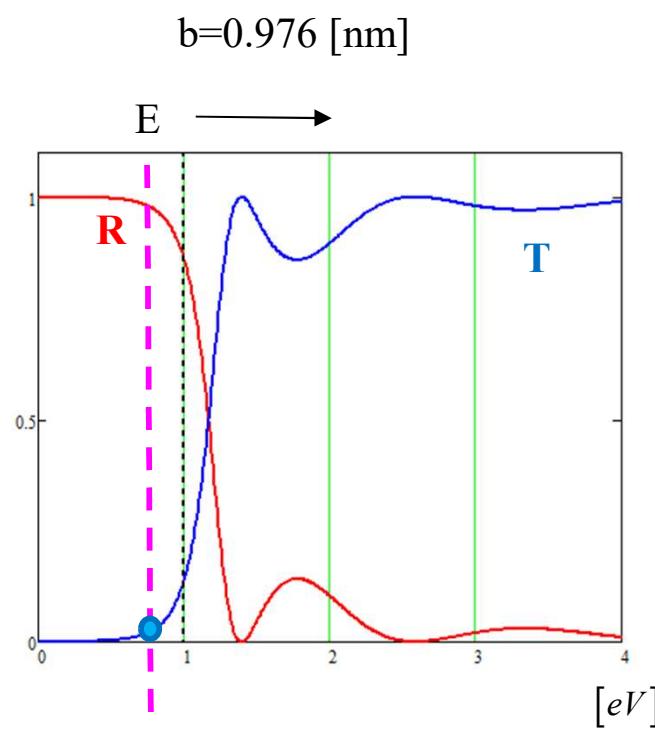
$$T = 1 - R$$



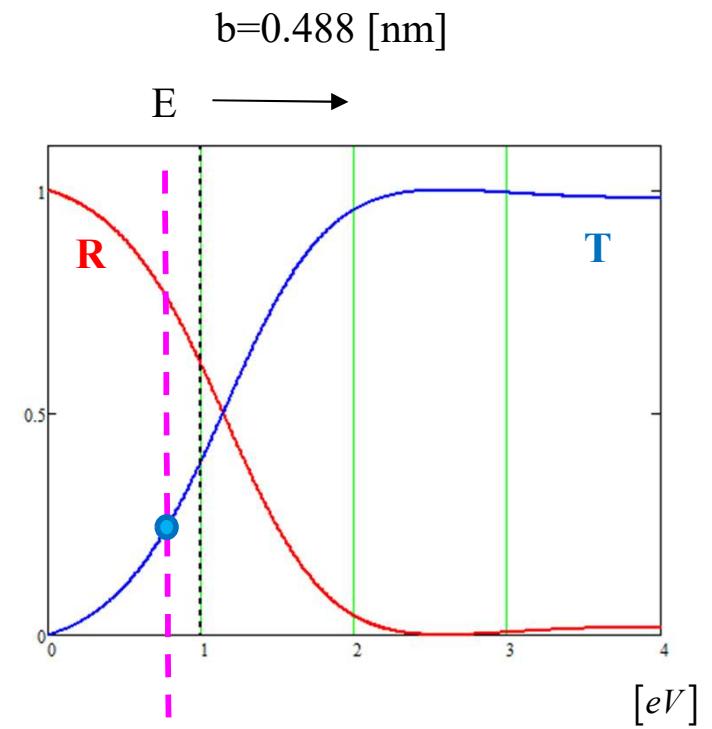
Effet tunnel



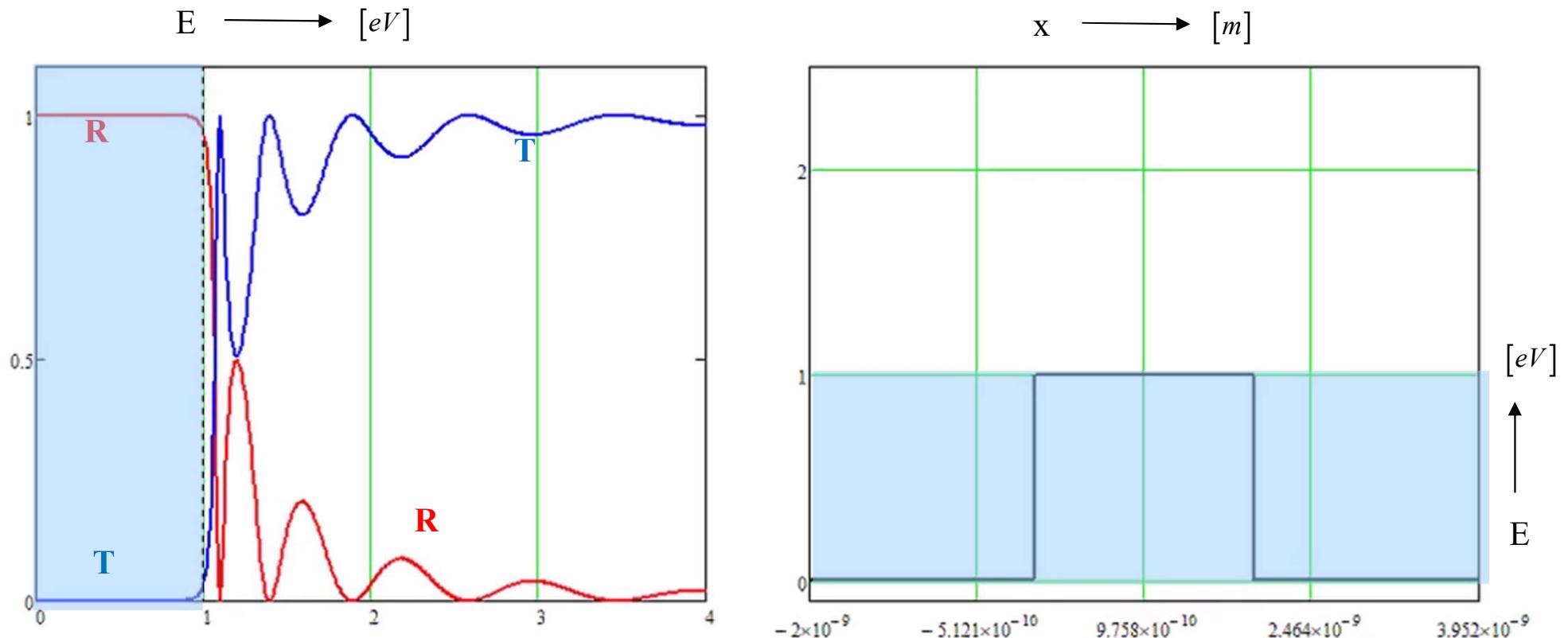
Barrière deux fois plus large



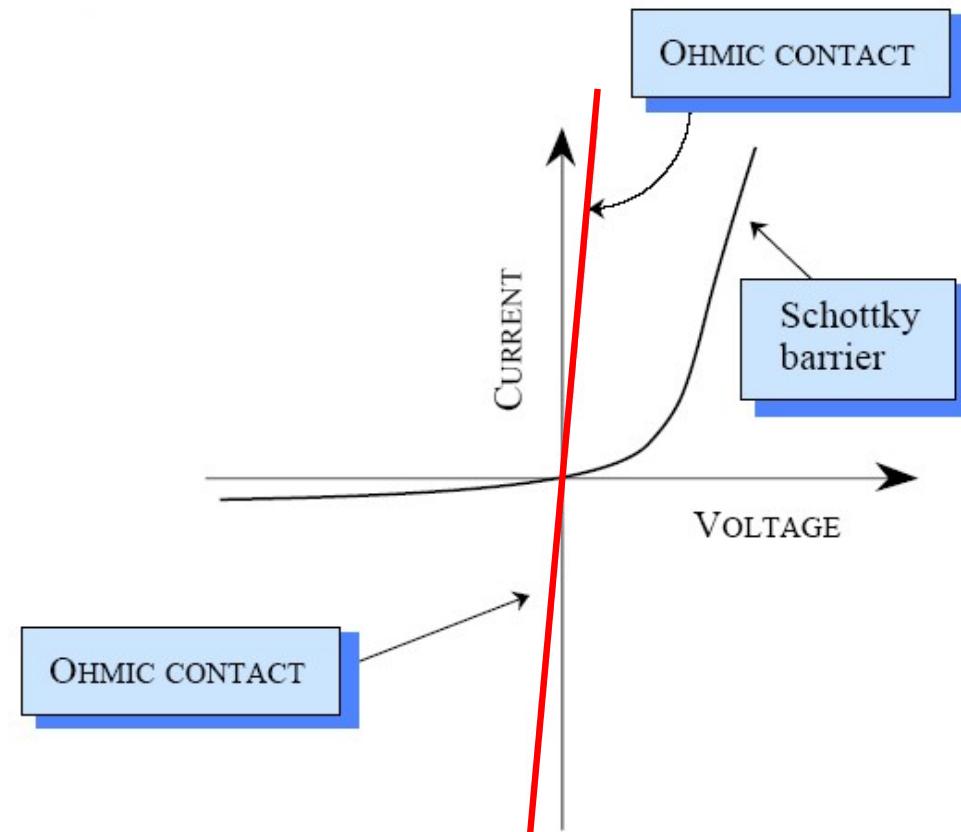
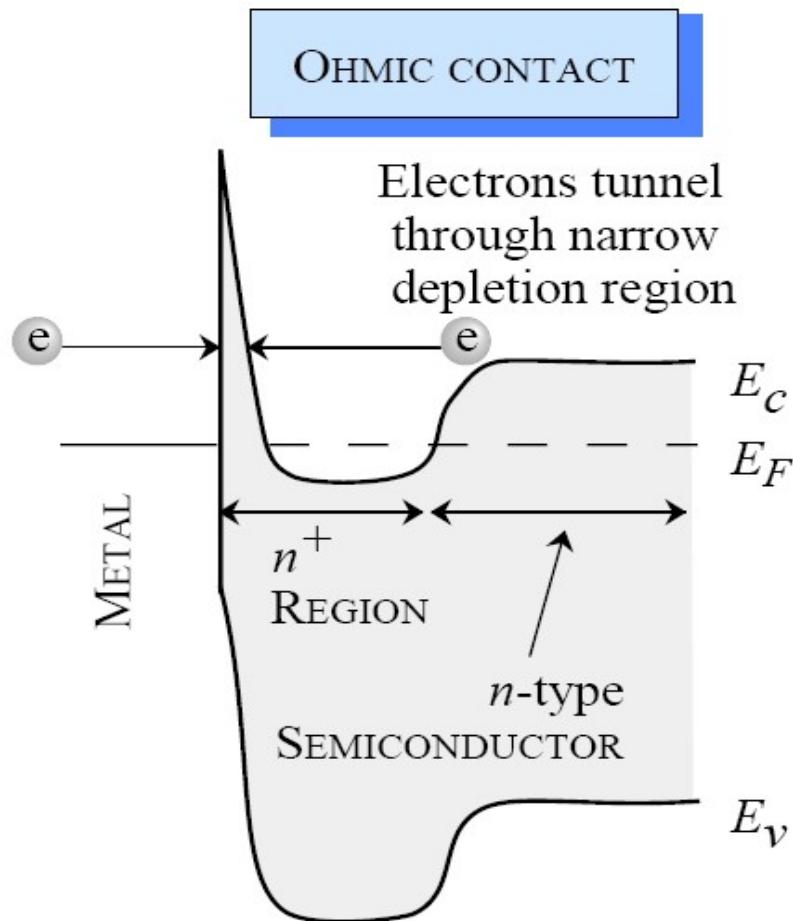
Barrière de référence



Barrière deux fois plus fine



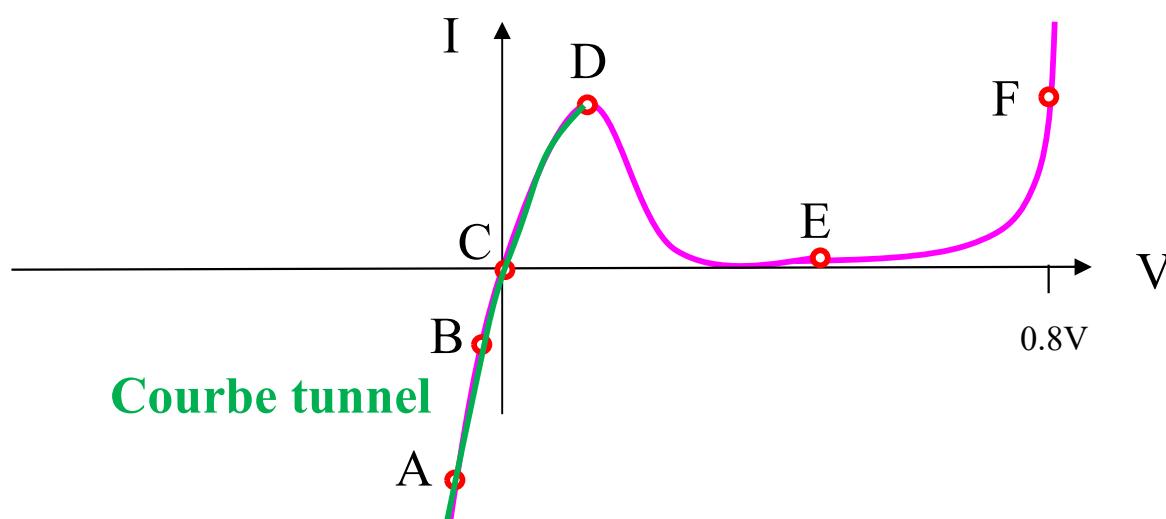
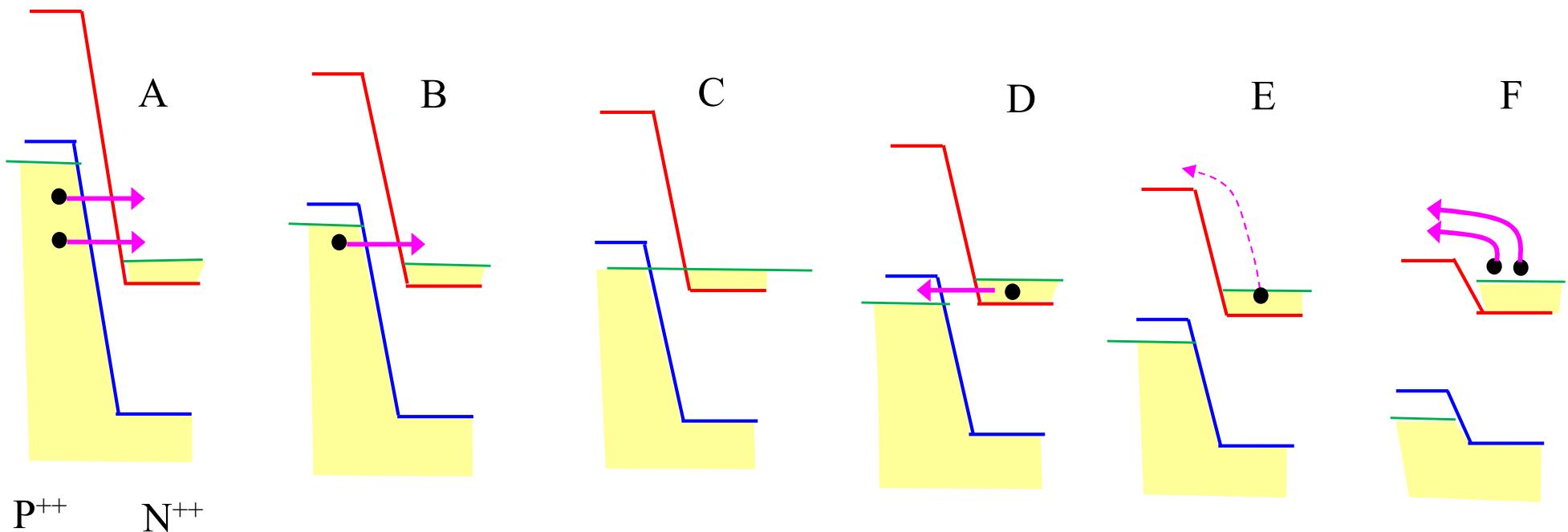
Effet tunnel (1) contact ohmique



J. Singh « *Semiconductor devices* »

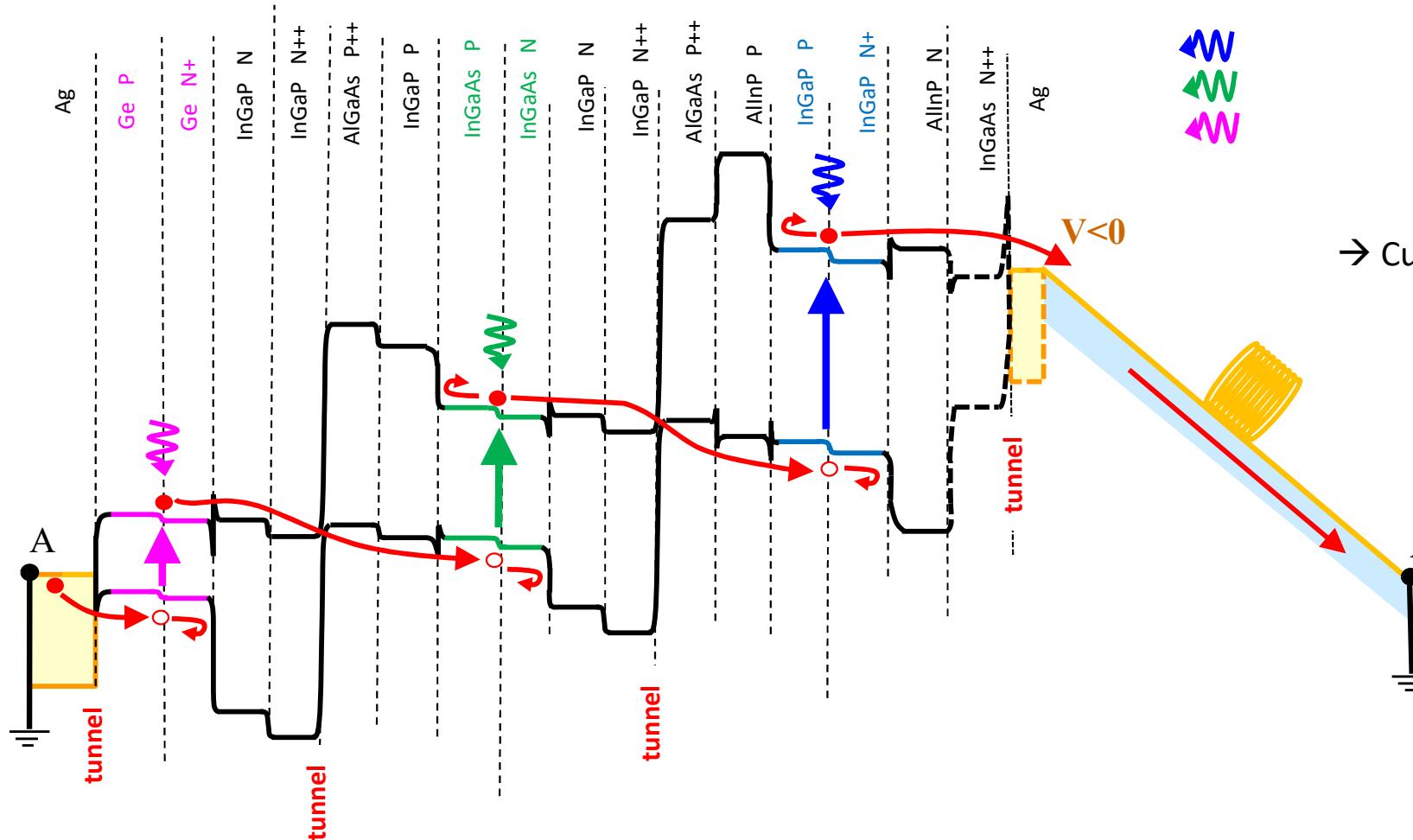
Effet tunnel (2) diode tunnel

L. Esaki, prix Nobel
de physique 1973



Effet tunnel (3) multi-junctions solar cells

BACK



FRONT

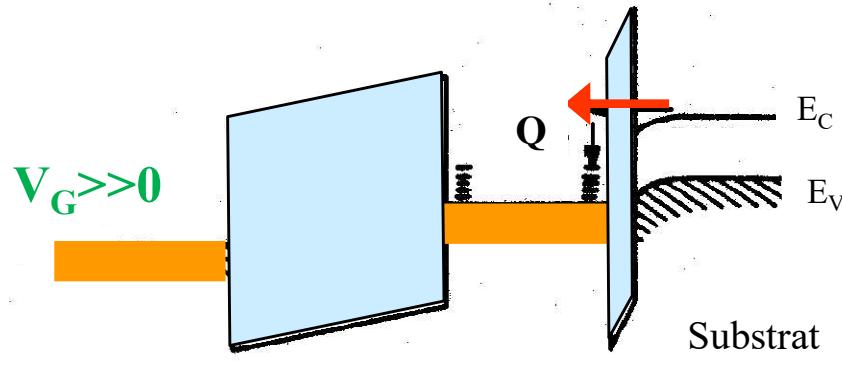
$$V = V_{bleu} + V_{vert} + V_{rouge}$$

$$I = \min[I_{bleu}, I_{vert}, I_{rouge}]$$

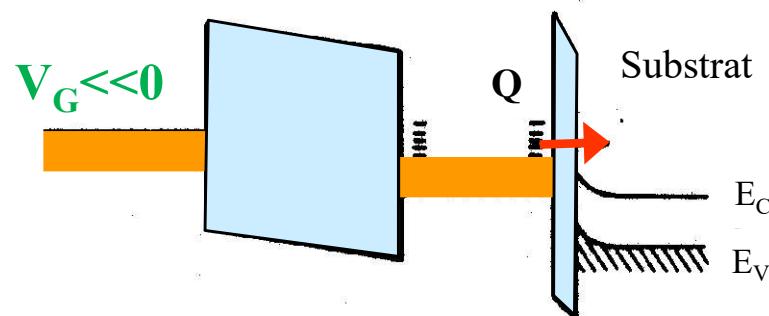
→ Current matching required



Effet tunnel (5) floating gate memories

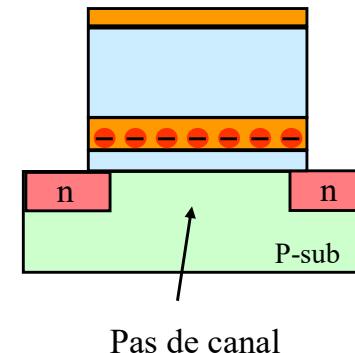


Écriture: $V_G \gg 0$



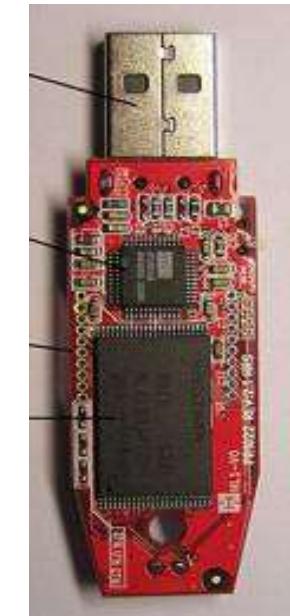
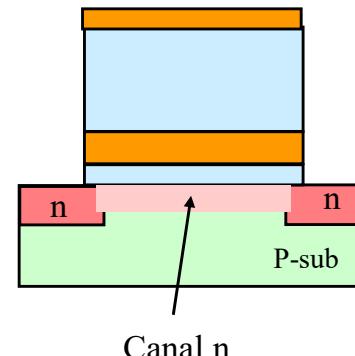
Effacer: $V_G \ll 0$

“1” state



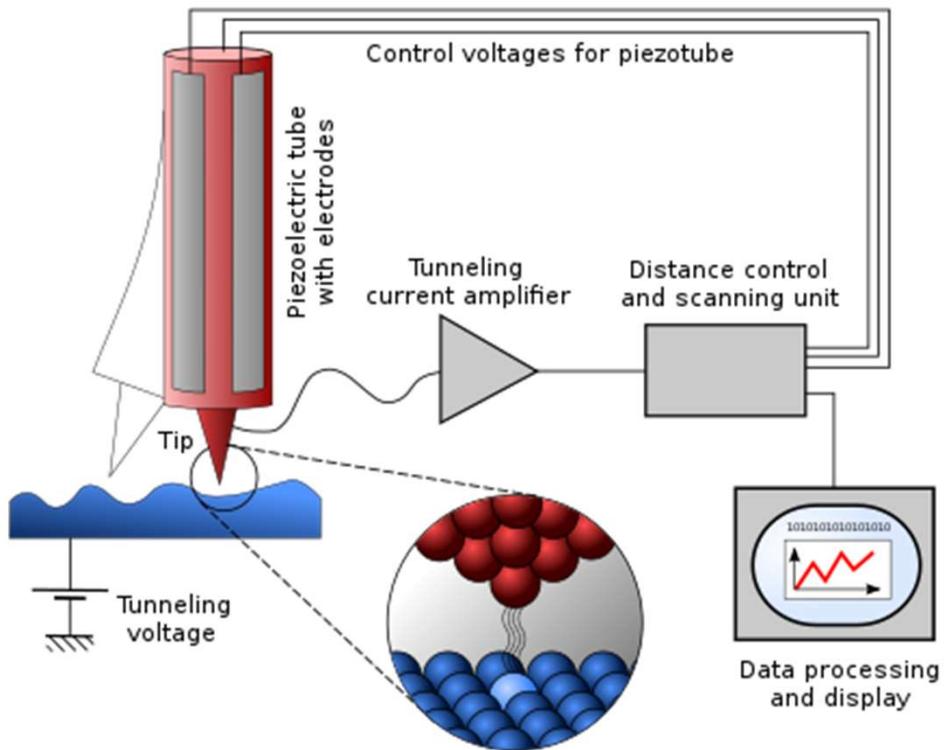
Pas de canal

“0” state



S. Sze « Physics of semiconductor devices »

Scanning tunneling microscope (STM)



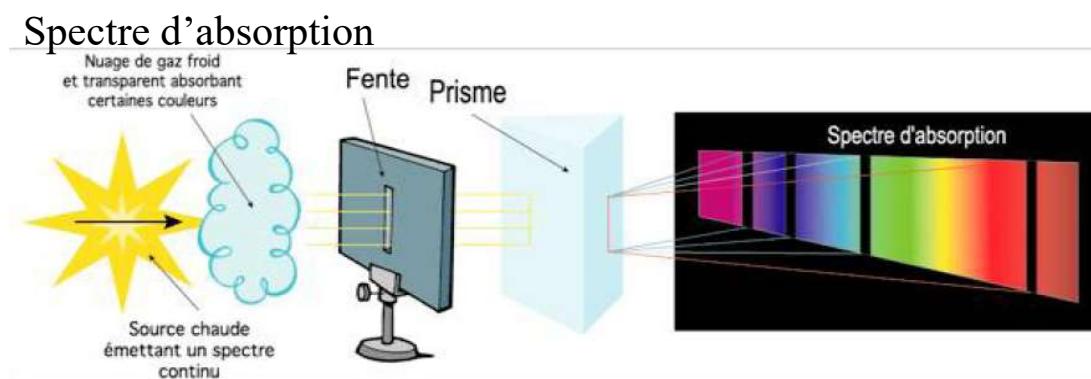
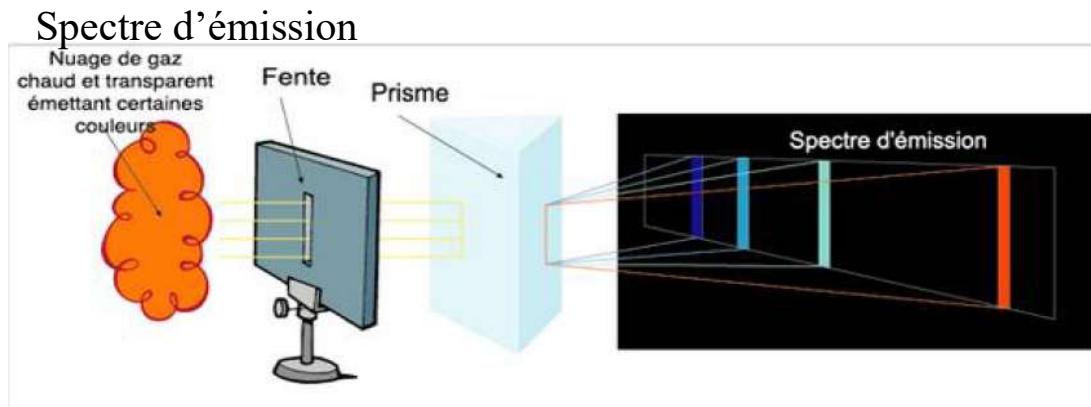
https://en.wikipedia.org/wiki/Scanning_tunneling_microscope

<https://www.nanoscience.com/techniques/scanning-tunneling-microscopy/>

Puits de potentiel

Atomes

Spectres d'émission et d'absoption

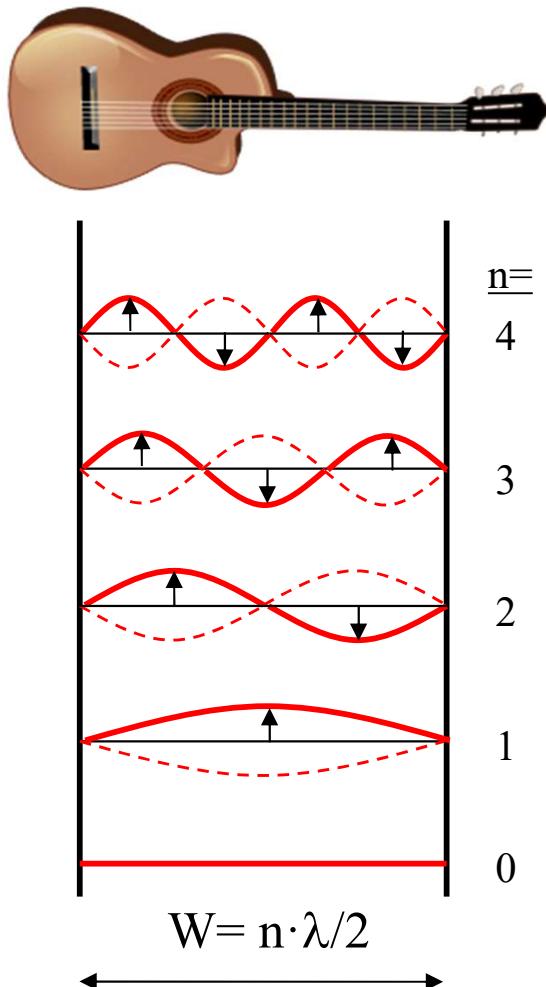


Les atomes ont des niveaux d'énergie discrets !

Ondes stationnaires

$$E = \frac{P^2}{2m} = \frac{\hbar^2 K^2}{2m}$$

$$E = n^2 \frac{\hbar^2 \pi^2}{2m W^2}$$



$$n =$$

$$3$$

$$2$$

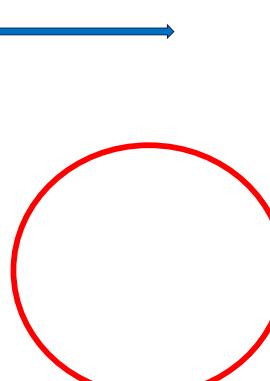
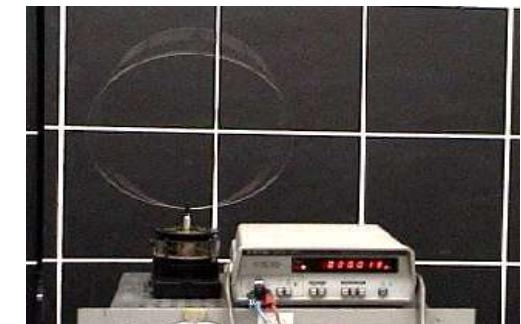
$$1$$

$$0$$

$$L = 2 \cdot \lambda$$

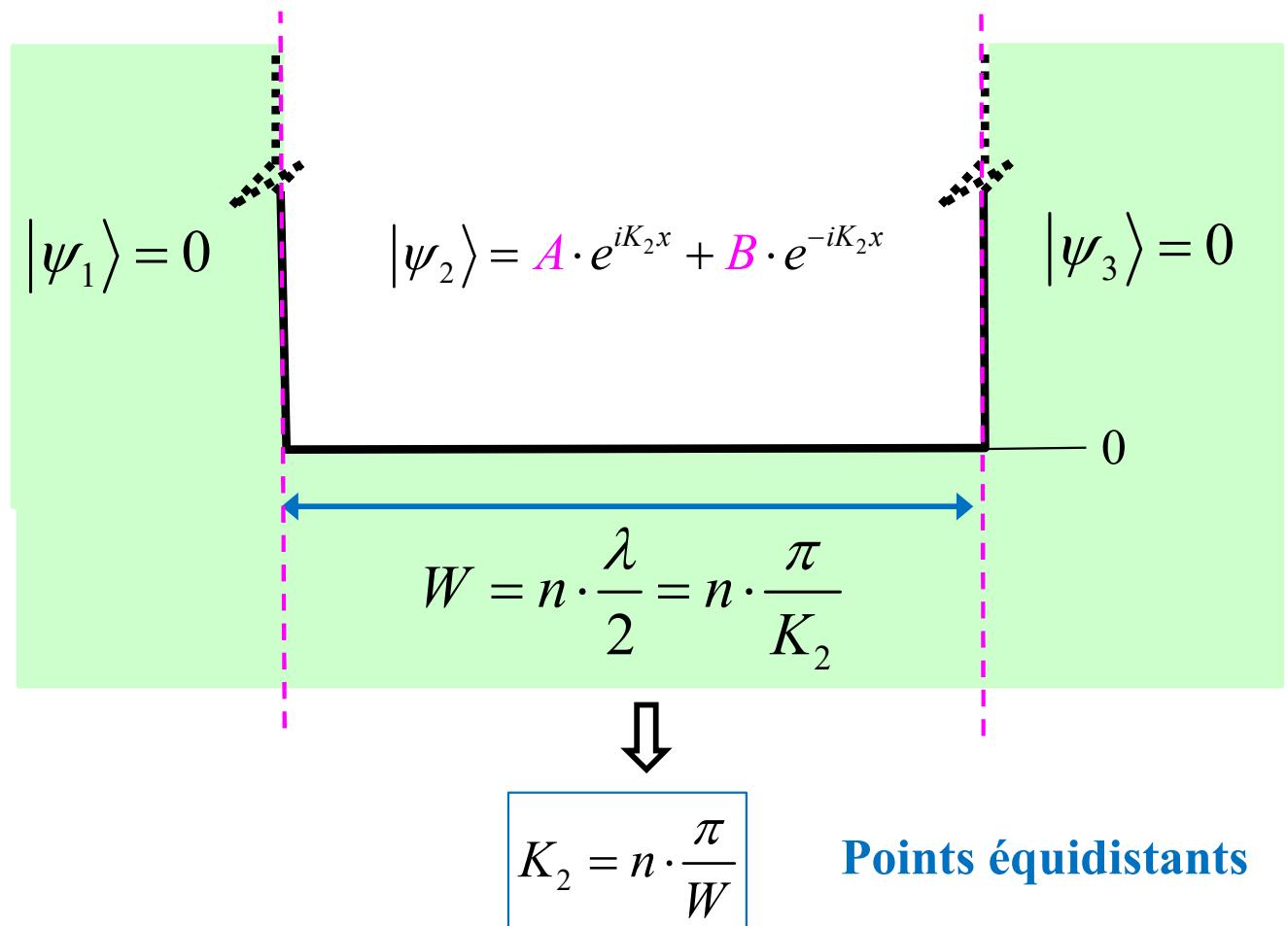
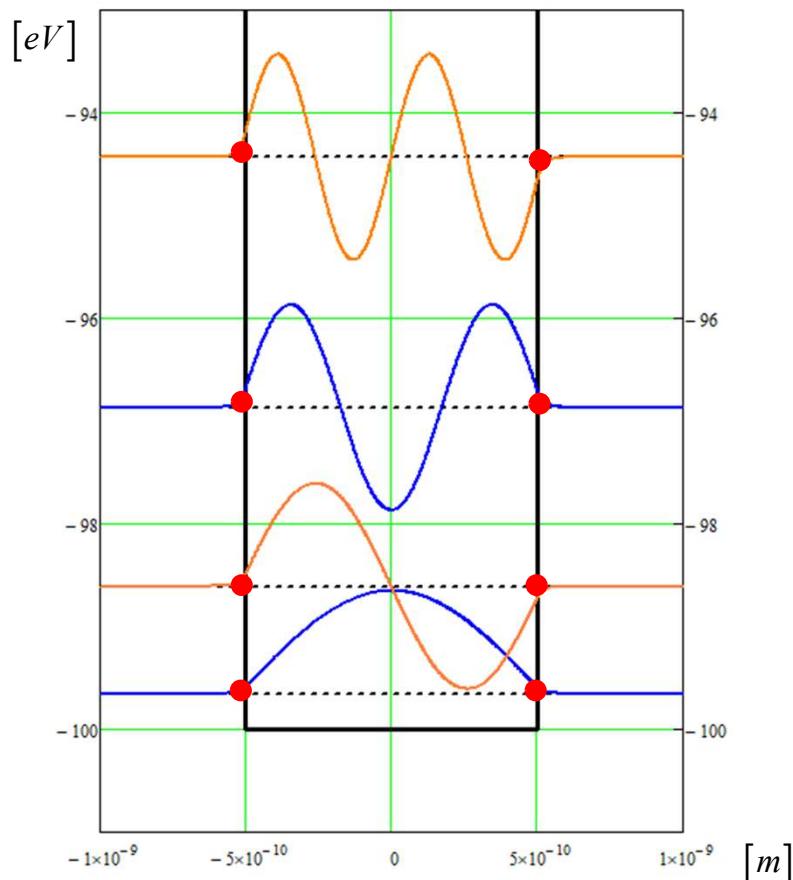
$$L = \lambda$$

Saint Mary's University



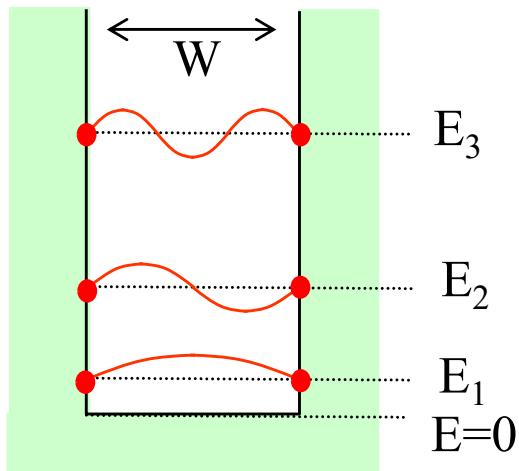
Potentiel rectangulaire

Puits quantique infini 1D



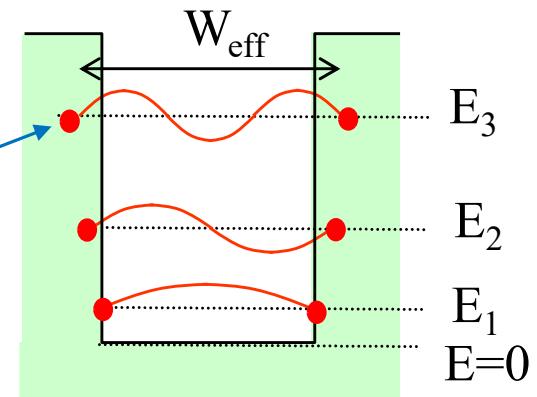
$$E_n = \frac{\hbar^2}{2m} K_2^2 = \left(\frac{\pi^2 \hbar^2}{2m \cdot W^2} \right) \cdot n^2$$

Puits infini



Puits fini

Ondes évanescentes



$$n \frac{\lambda}{2} = W$$

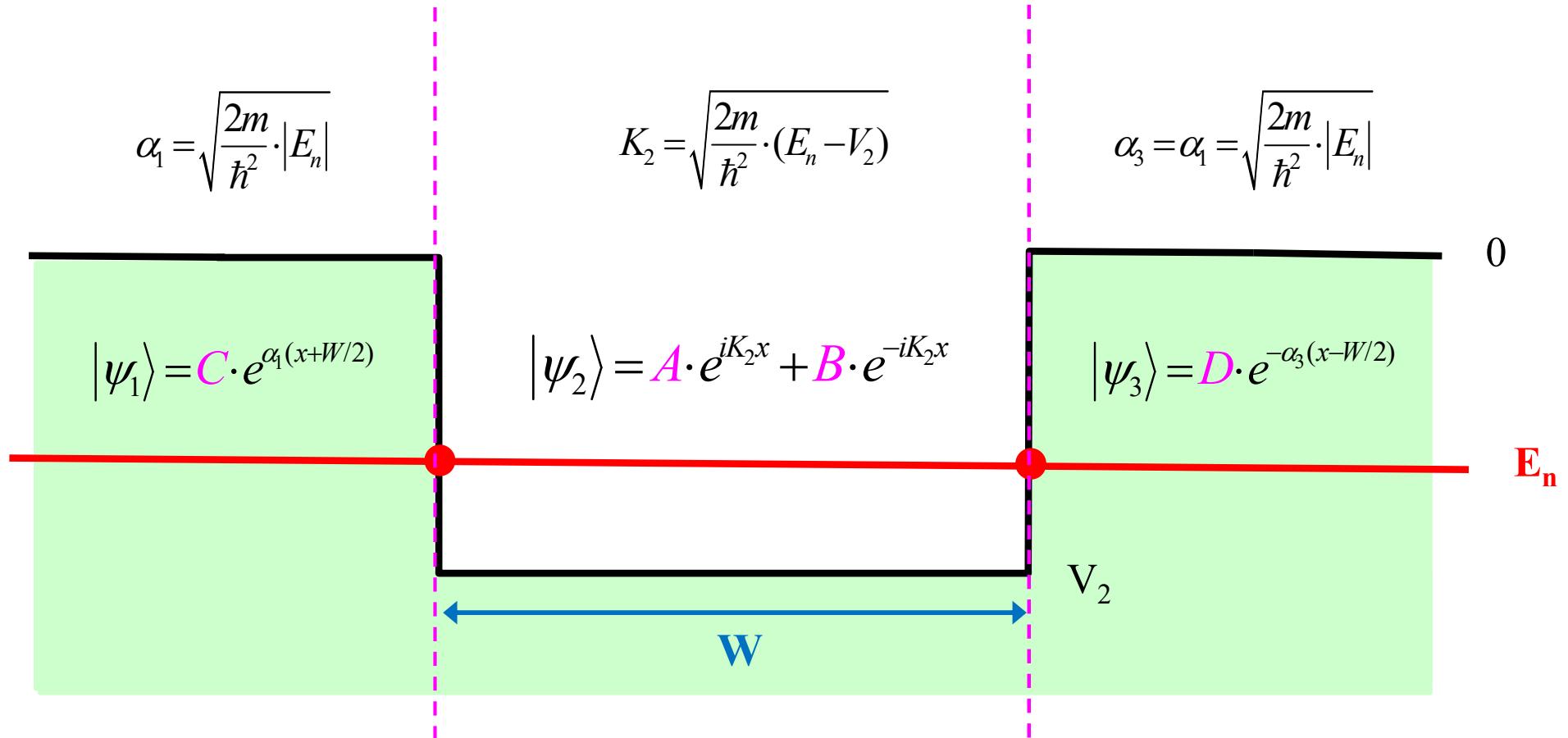
Pénétration latérale
surtout pour états supérieurs

$$E_n = \frac{\hbar^2 K^2}{2m} = n^2 \cdot \frac{\hbar^2 \pi^2}{2m W^2}$$

« Etats discrets »

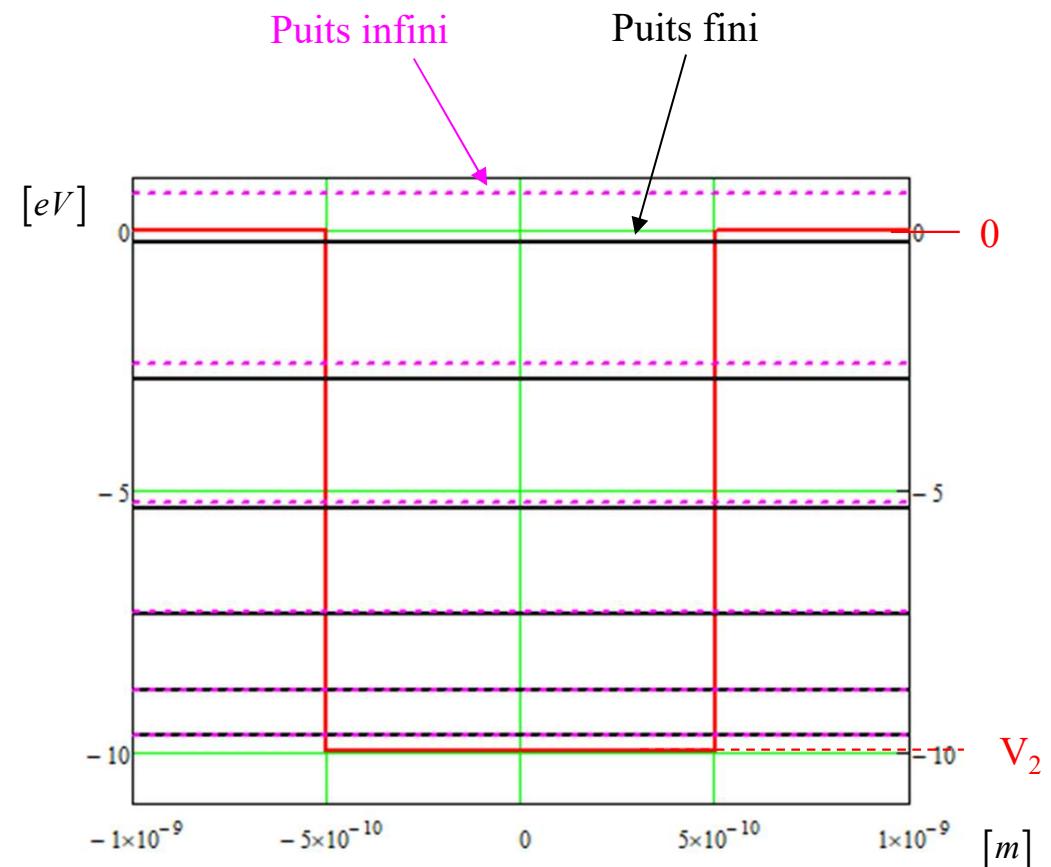
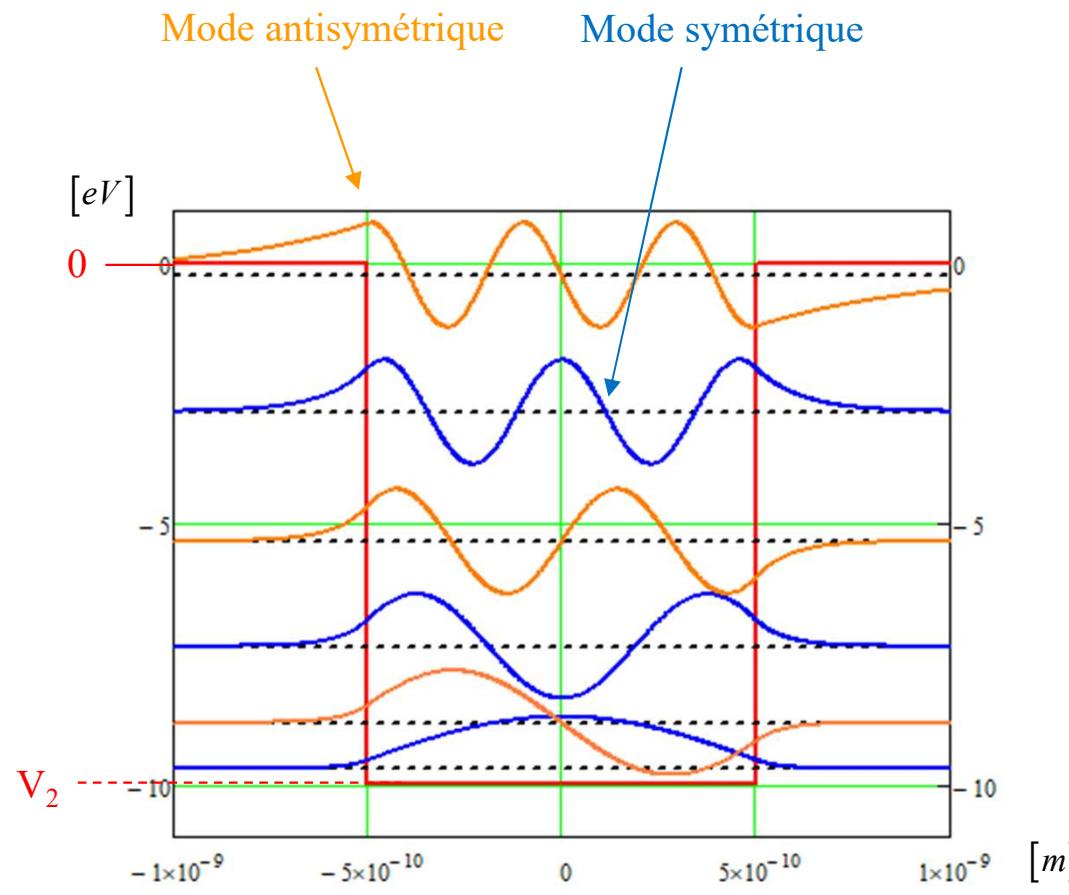
$$E_n \cong n^2 \cdot \frac{\hbar^2 \pi^2}{2m W_{\text{eff}}^2}$$

Puits quantique fini, 1D

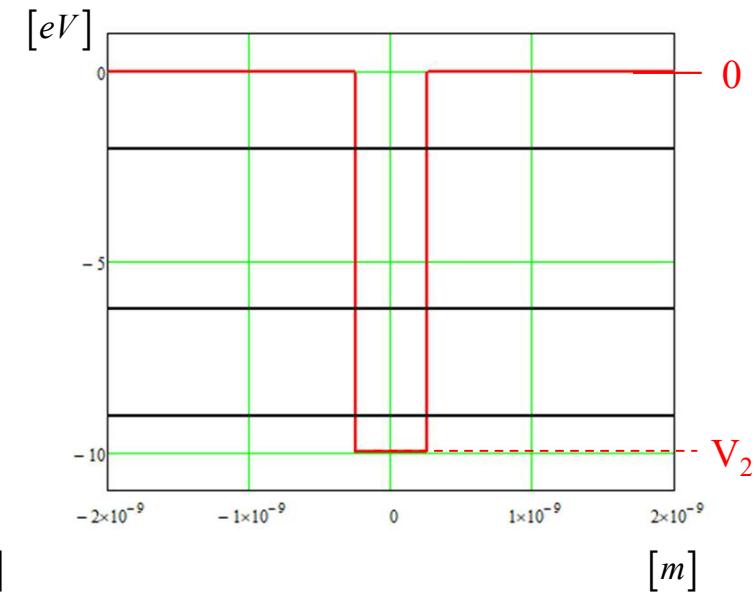
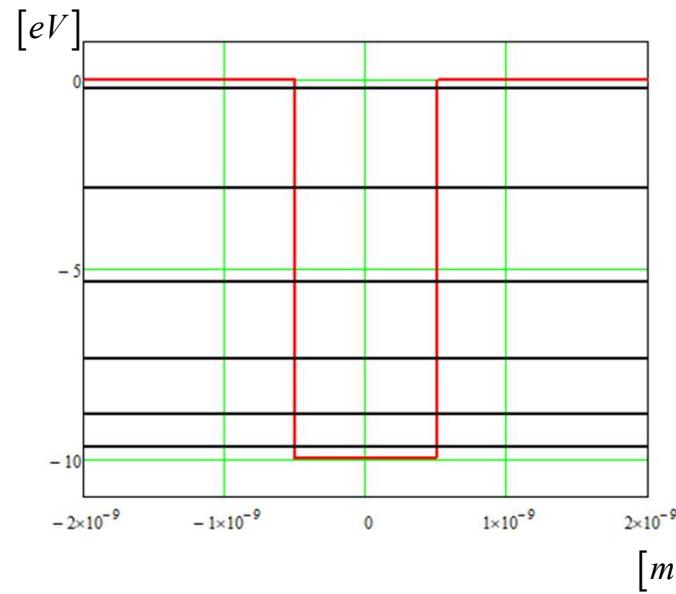
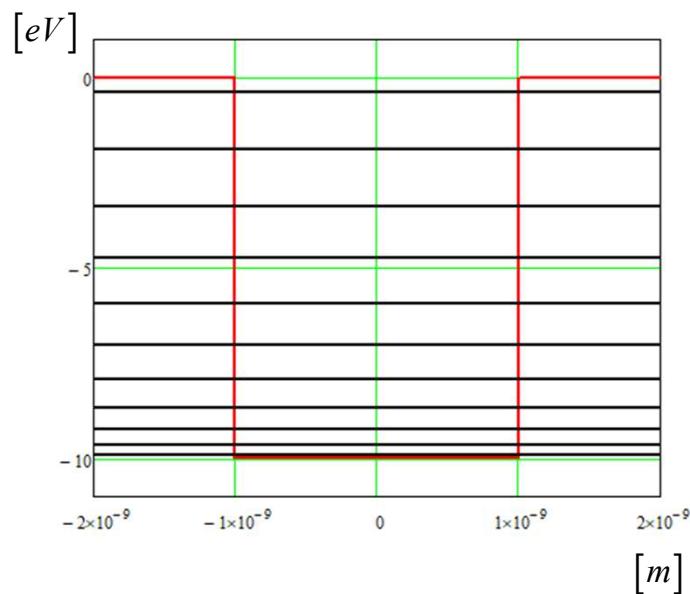


Aux interfaces, la fonction d'onde et sa dérivée sont continues
 → déterminer A,B,C,D et E_n

Puits de potentiel



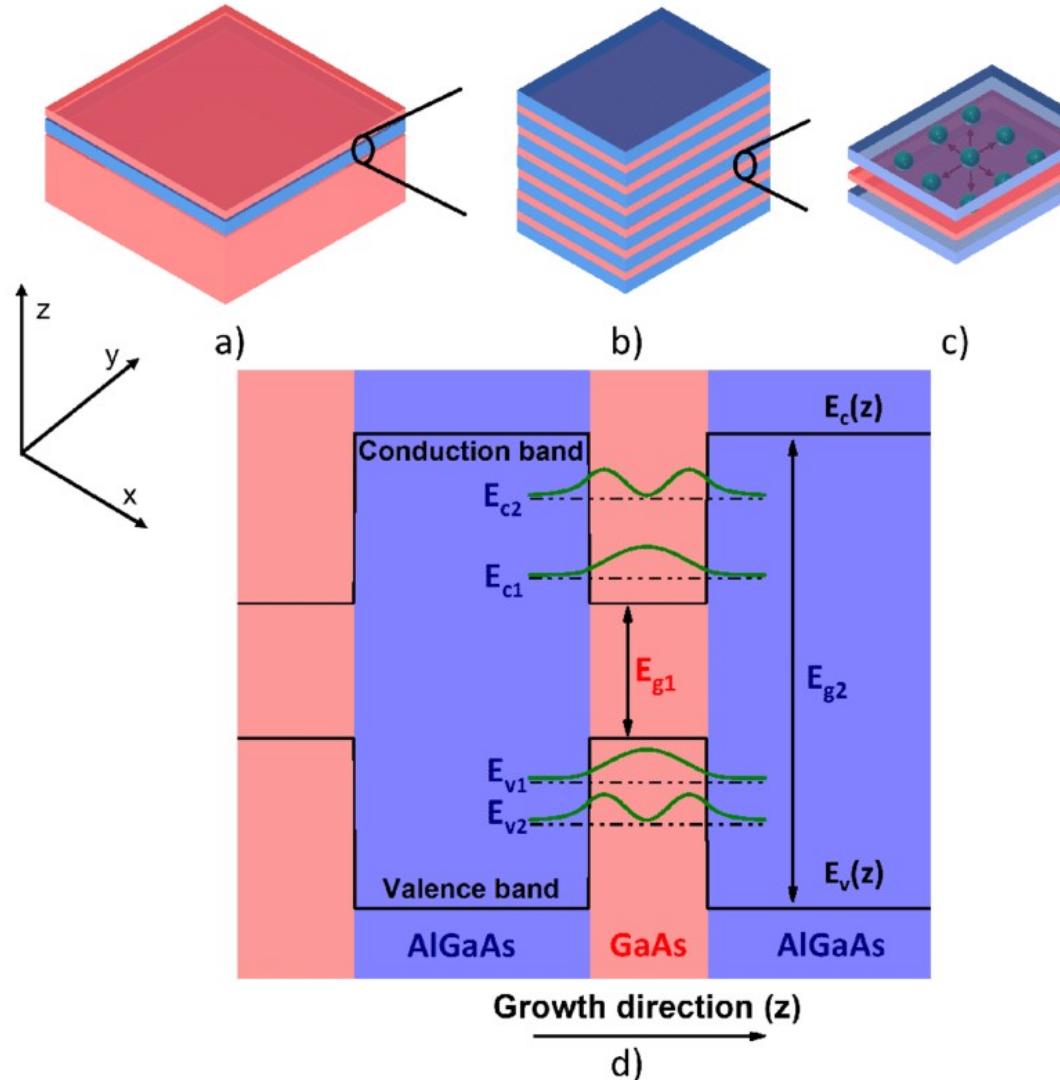
Puits de potentiel



$$E_n - V_2 \approx n^2 \cdot \frac{1}{W_{eff}^2}$$

Quantum Wells

https://www.researchgate.net/publication/348894632_Mid-Infrared_Intersubband_Polaritonic_Devices

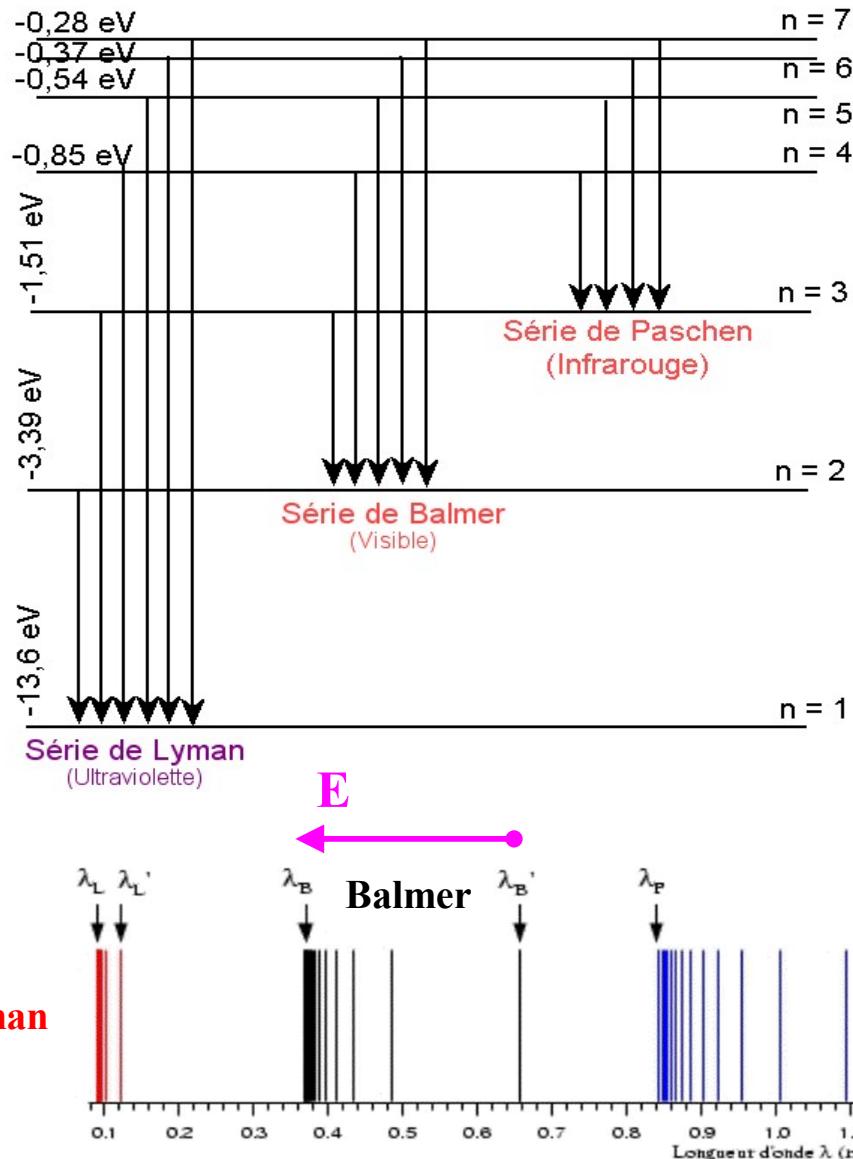


2D electron gas

- K_z discret
- K_x et K_y continu

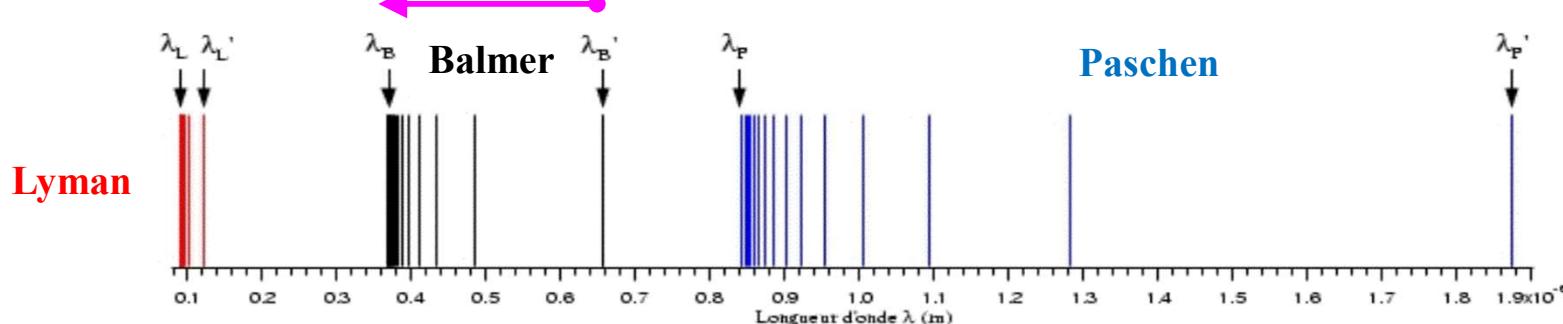
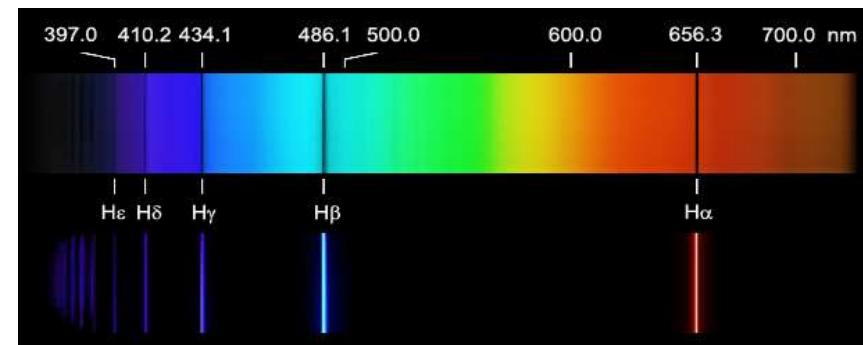
Potentiel de Coulomb et Atome d'hydrogène

Spectre de l'hydrogène



[http://physiquereussite.fr/latome2/
spectre-hydrogène-balmer/](http://physiquereussite.fr/latome2/spectre-hydrogène-balmer/)

Série de Balmer en visible

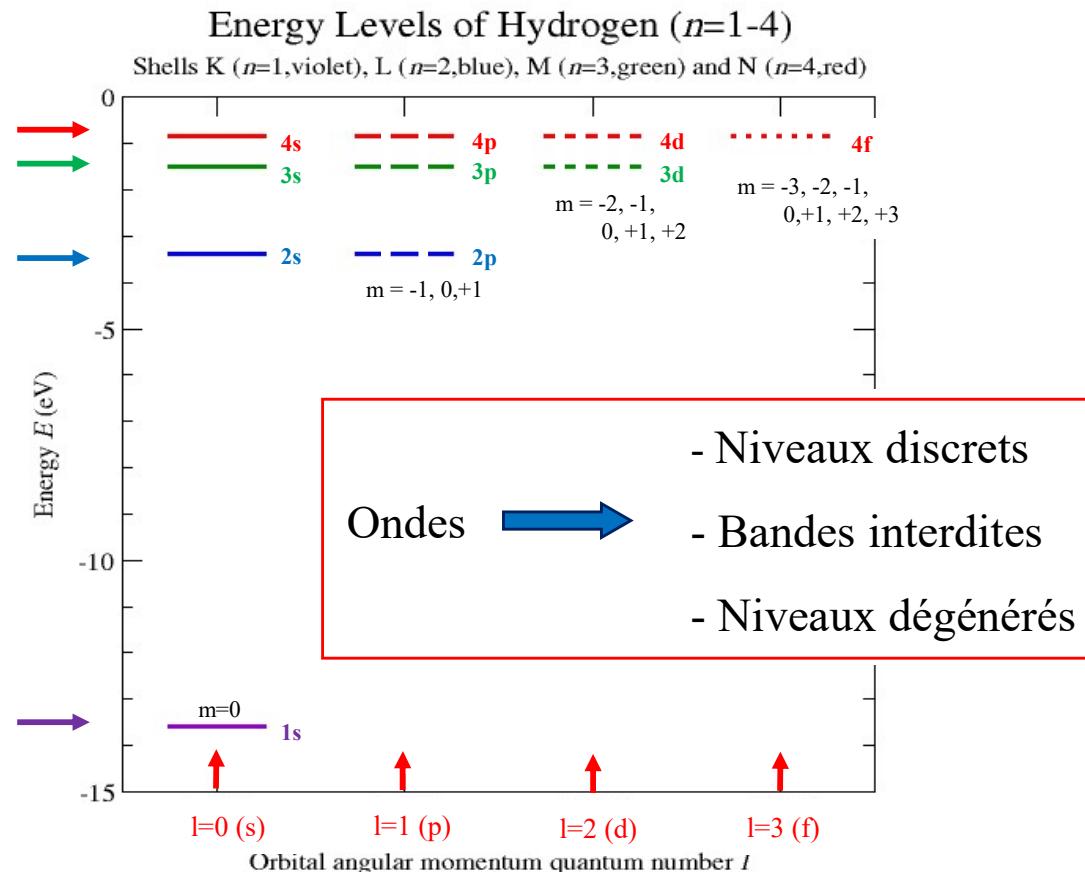


Niveaux d'énergie de l'hydrogène

$$E_n = -13.6 \cdot \frac{1}{n^2} \quad [eV]$$

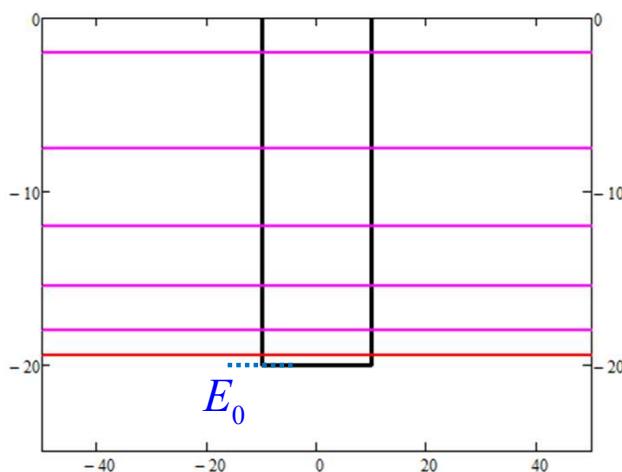
n=1

n=2
n=3
n=4

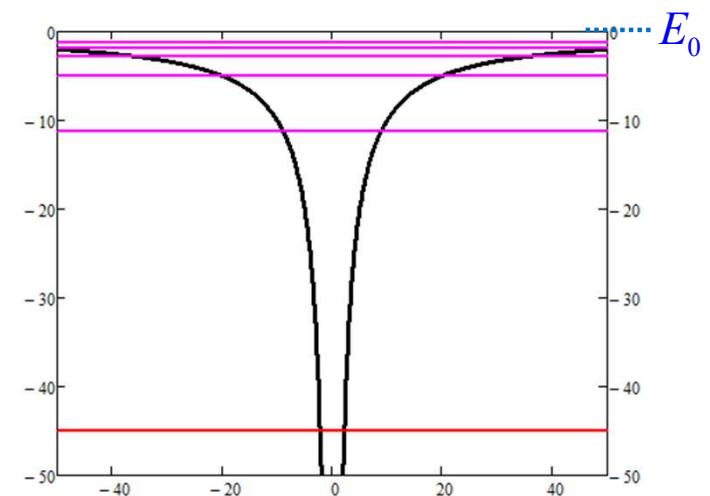


http://en.wikipedia.org/wiki/Laplace-Runge-Lenz_vector

Potentiel rectangulaire



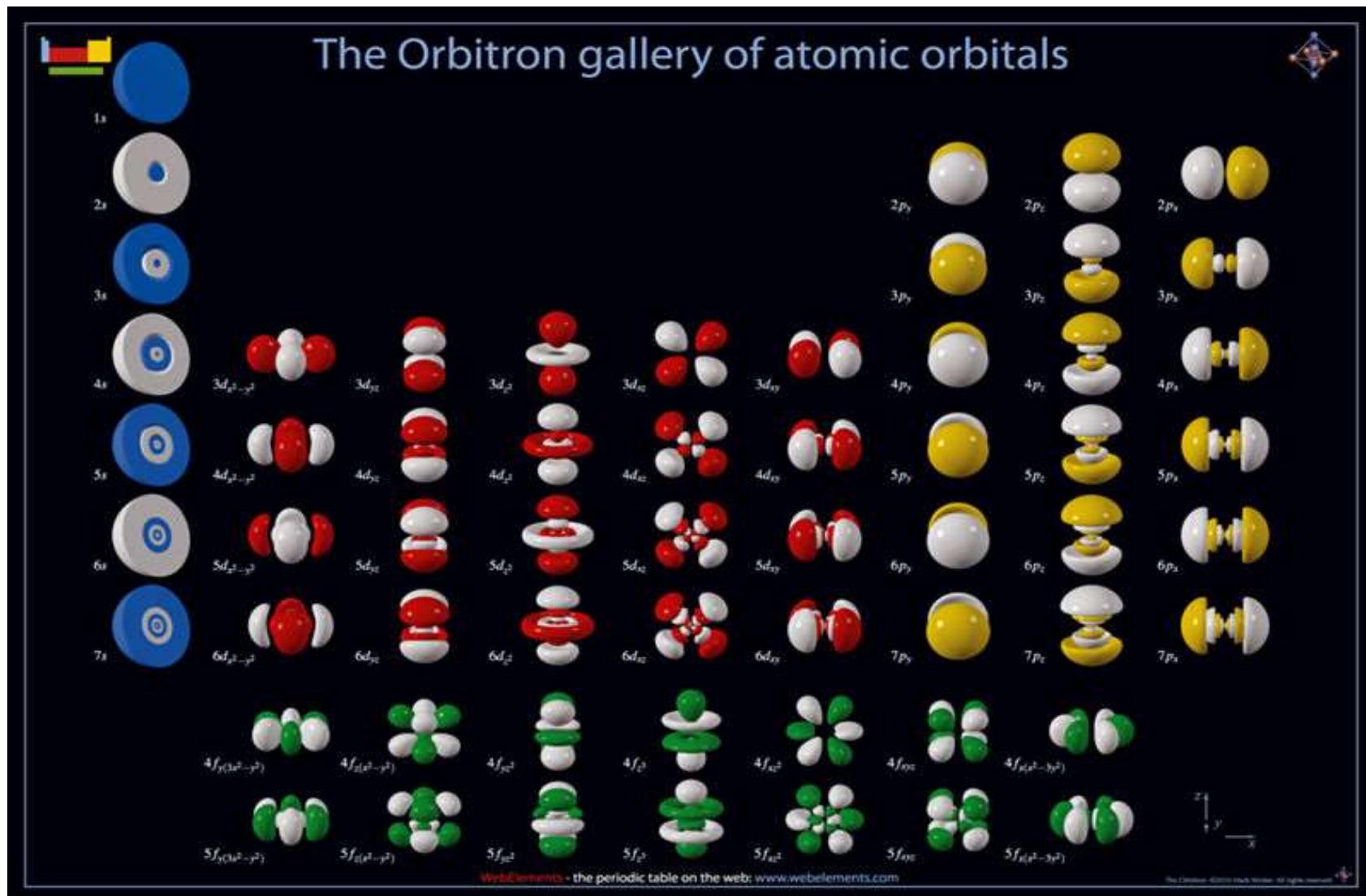
Potentiel en $1/r$



$$E_n - E_0 \approx \frac{n^2}{W^2}$$

$$E_n - E_0 \approx -\frac{1}{n^2}$$

Orbitales atomiques



www.webelements.com/shop/

Potentiel quadratique et Oscillateur harmonique

Vibrations cristallines («phonons»):

Oscillations de l'énergie cinétique à l'énergie potentielle

$$H = \frac{1}{2m} P^2 + \frac{\kappa}{2} X^2$$

Ondes électromagnétiques («photons»):

Oscillations de l'énergie du champ E et celle du champ B

$$H = \frac{\epsilon_0}{2} |E|^2 + \frac{1}{2\mu_0} |B|^2$$

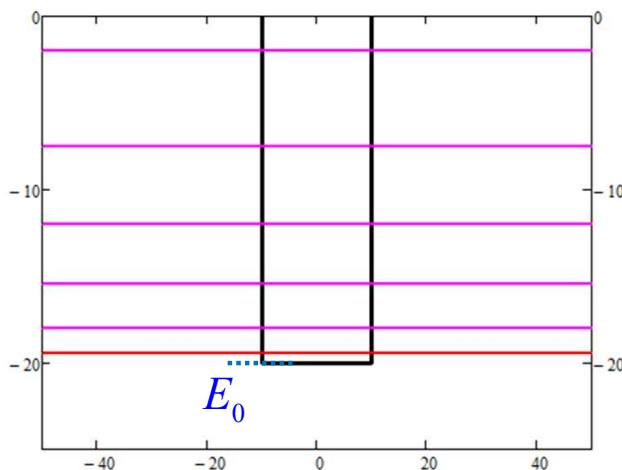
Résonateurs LC:

Oscillations de l'énergie dans la capacité et celle dans l'inductance

$$H = \left(\frac{1}{2C} Q^2 \right) + \left(\frac{1}{2L} \phi^2 \right)$$

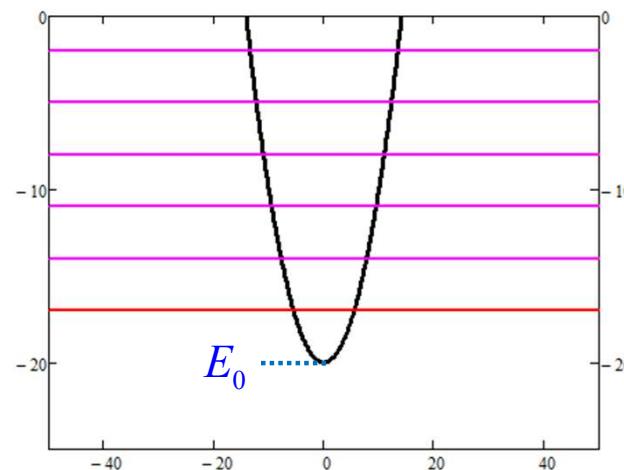
Formes du potentiel

Potentiel rectangulaire



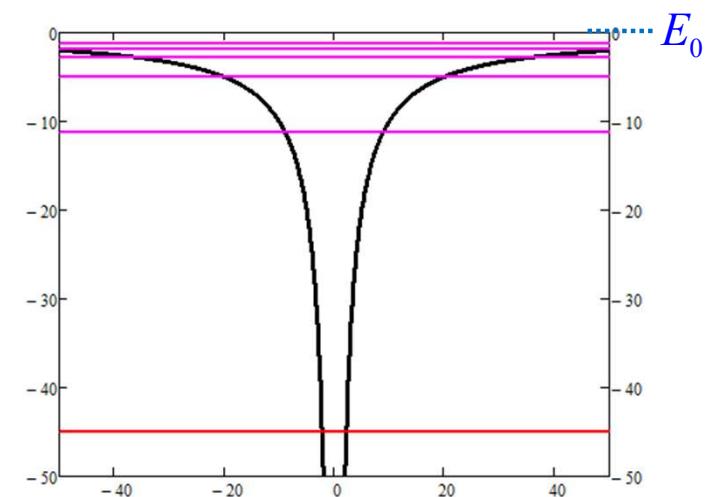
$$E_n - E_0 \approx n^2$$

Potentiel quadratique



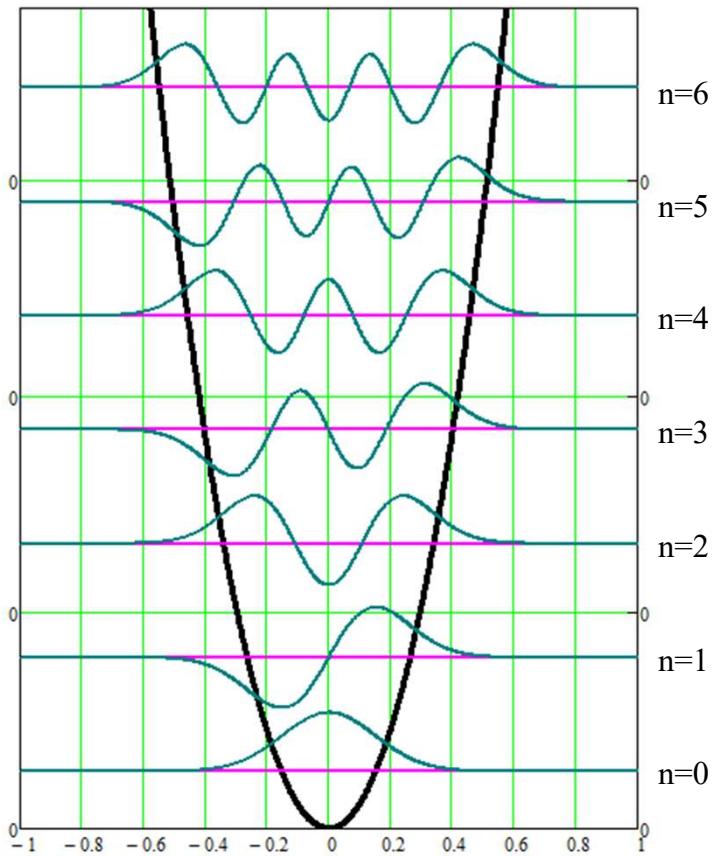
$$E_n - E_0 \approx n$$

Potentiel en 1/r



$$E_n - E_0 \approx -\frac{1}{n^2}$$

Oscillateurs harmoniques quantiques



Modes propres de l'équation de Schroedinger:

$$i\hbar \cdot \frac{\partial}{\partial t} |\psi_n\rangle = E_n \cdot |\psi_n\rangle = \frac{\hbar\omega}{2} \cdot (P^2 + Q^2) \cdot |\psi_n\rangle$$

Energie
cinétique



Energie
potentielle

$$E_n = \hbar\omega \cdot \left(n + \frac{1}{2} \right)$$

$$|\psi_n\rangle = A_n \cdot e^{-\frac{Q^2}{2}} \cdot H_n(Q)$$

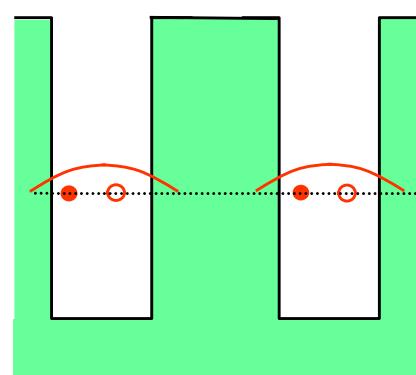
Polynômes
Hermite

Couplage de puits

Molécules

Deux atomes: états liants et anti-liants

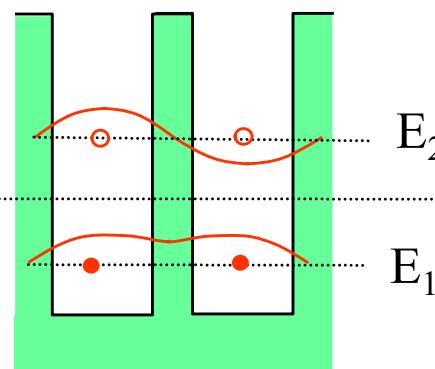
Deux atomes séparés
avec 1 électron chacun



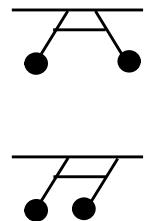
Hybridation

E_0

Deux atomes proches
avec 1 électron chacun



Anti-liant
Liant



Deux états identiques:

- localisés
- deux spins possibles par état
- un électron dans chaque puits

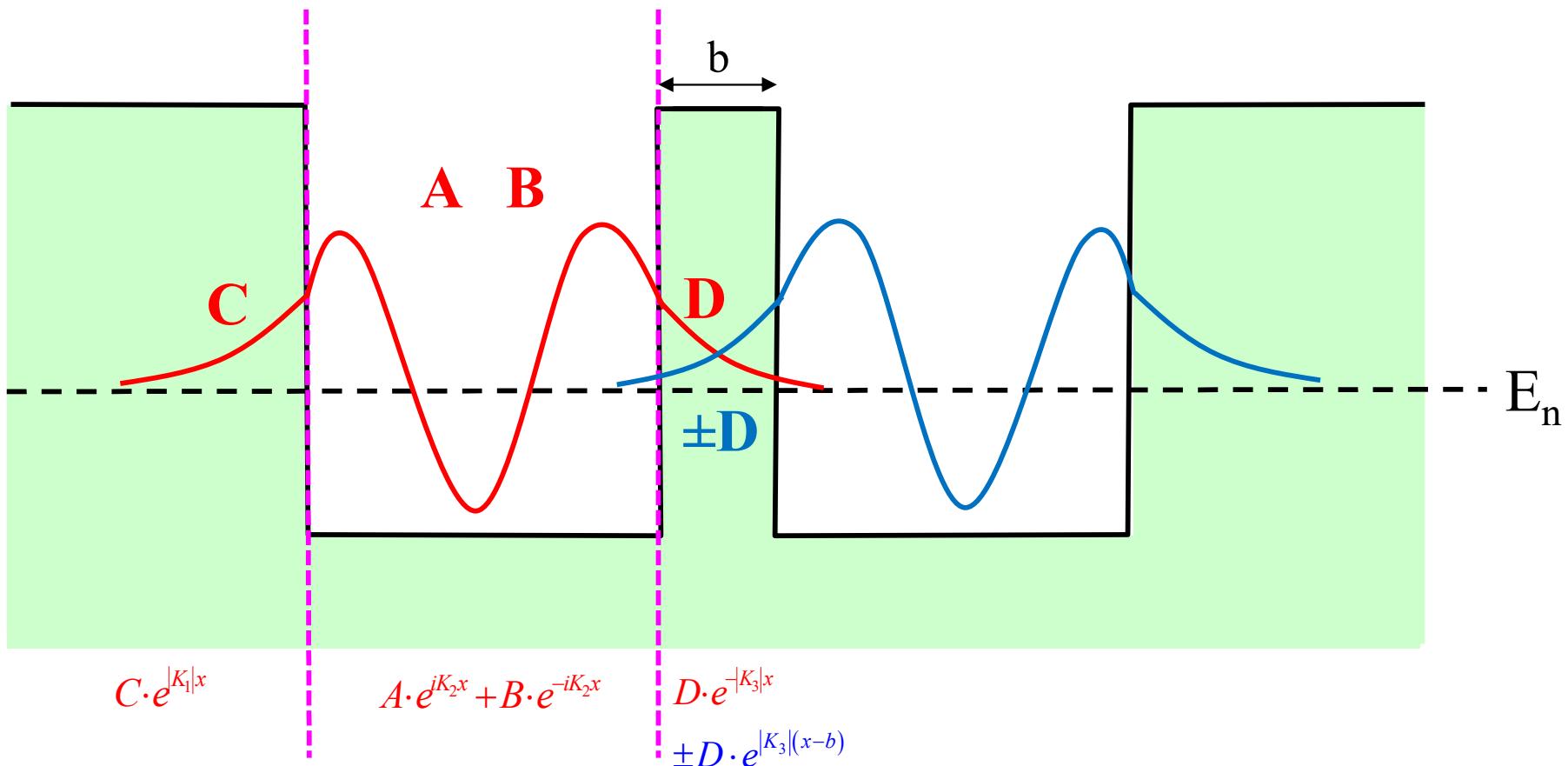
Etat « liant »:

- énergie profonde, occupé par un électron de chaque atome.

Etat « anti-liant »:

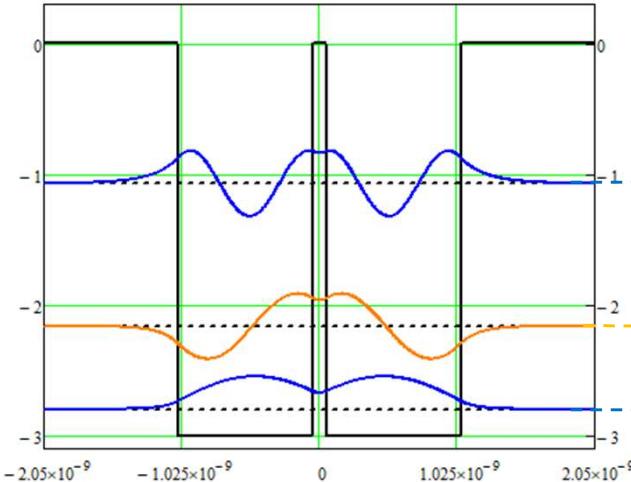
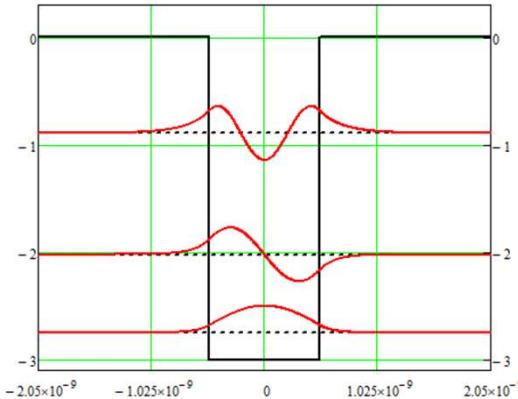
- énergie supérieure, libre à basse température

Calcul des fonctions d'ondes et des énergies pour deux puits couplés

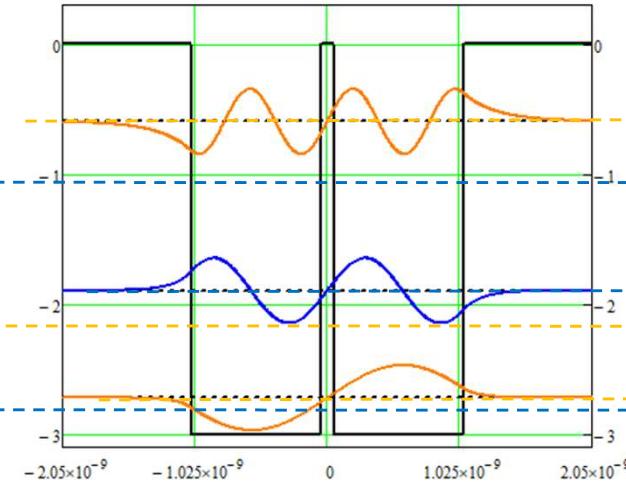


Aux interfaces, la fonction d'onde et sa dérivée sont continues
 → déterminer A,B,C,D et E_n

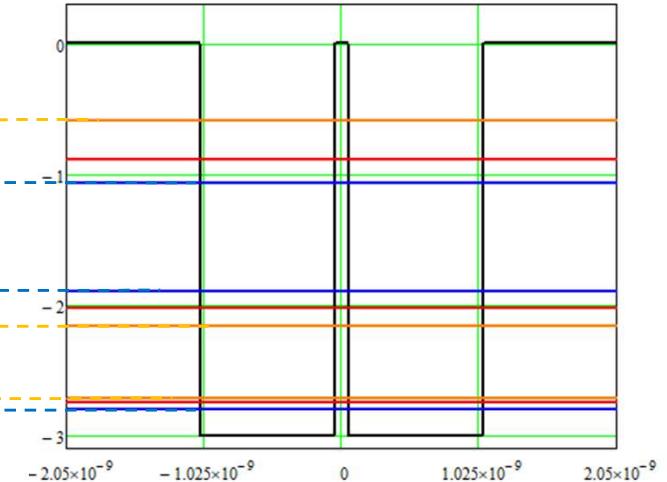
Double puits: couplage fort



Modes symétriques

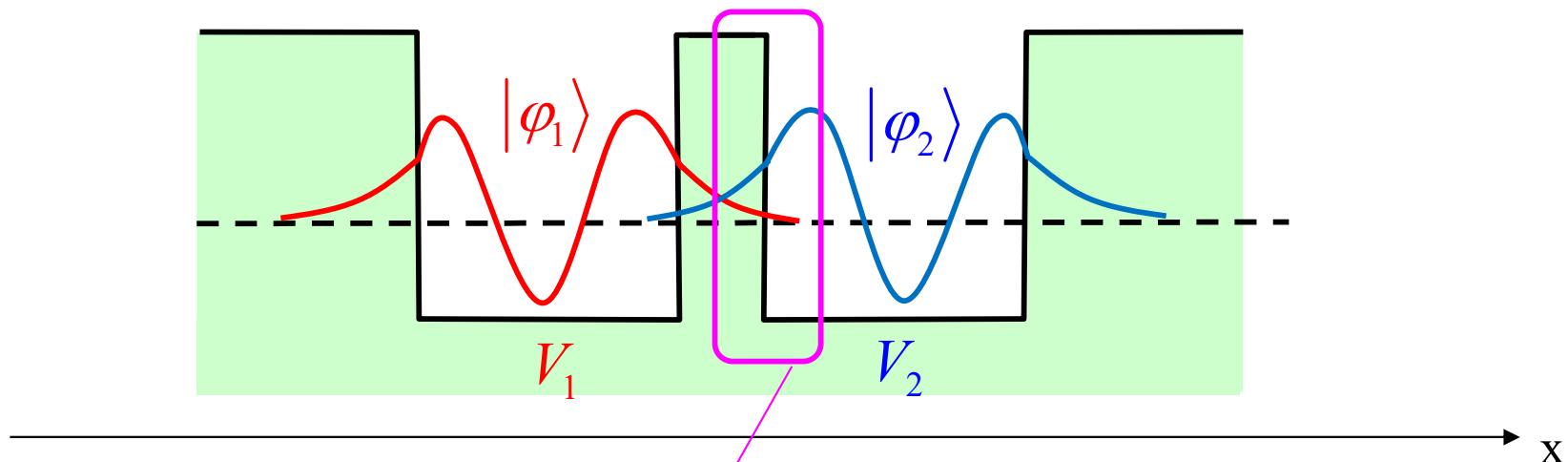


Modes asymétriques



Energies

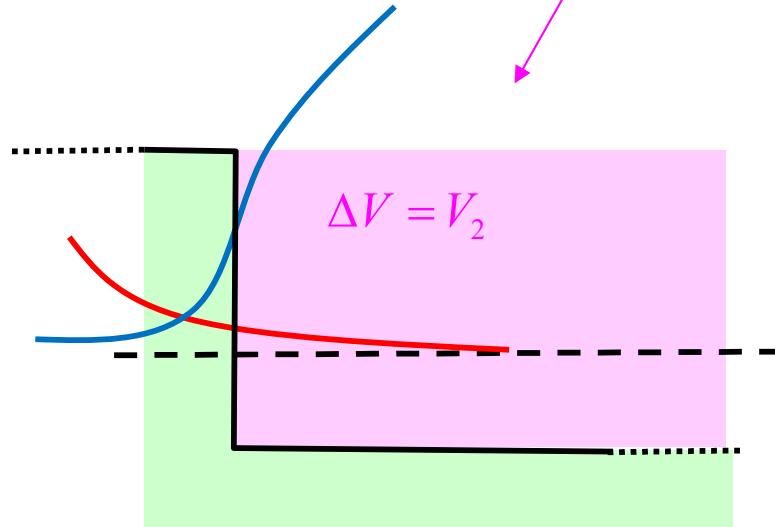
Théorie des perturbations



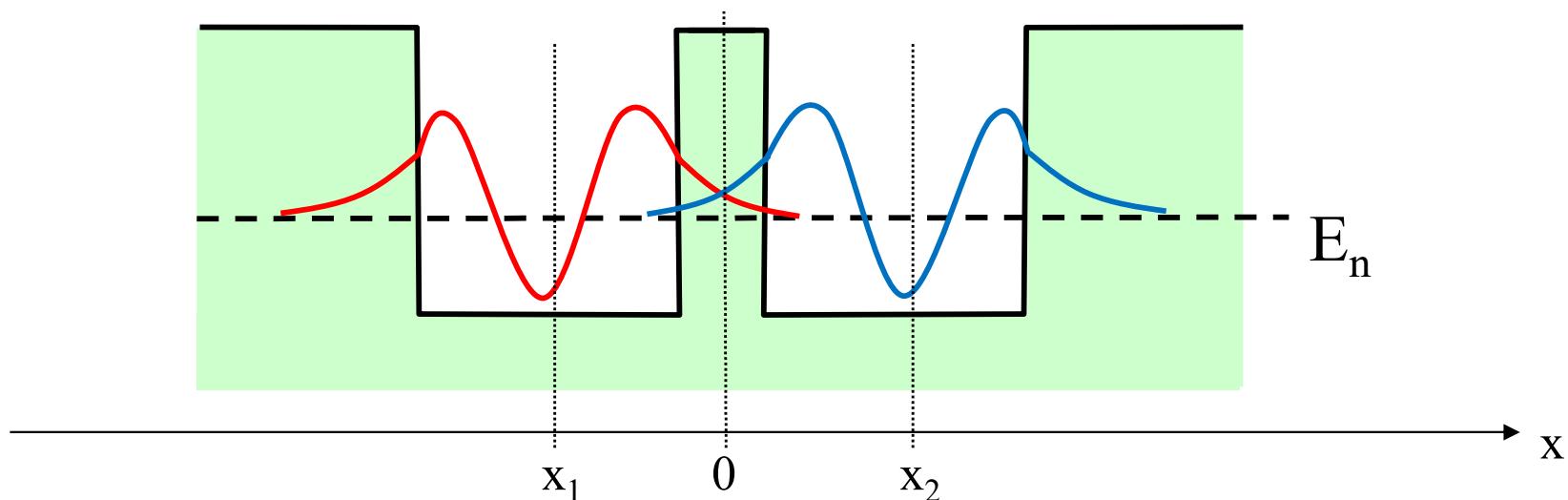
$$T_{12} = \langle \varphi_1 | E_0 + \Delta V | \varphi_2 \rangle$$

$$T_{11} = \langle \varphi_1 | \Delta V | \varphi_1 \rangle \ll T_{12}$$

$$H = \begin{pmatrix} E_0 + T_{11} & T_{12} \\ T_{12}^* & E_0 + T_{11} \end{pmatrix}$$



Deux puits couplés



$$|\psi(x,t)\rangle \cong \begin{pmatrix} \alpha_1(t) \\ \alpha_2(t) \end{pmatrix} \quad \begin{array}{ll} \leftarrow \langle \varphi(x-x_1) \middle\| \psi(x,t) \rangle & \text{«puits de gauche»} \\ \leftarrow \langle \varphi(x-x_2) \middle\| \psi(x,t) \rangle & \text{«puits de droite»} \end{array}$$

Théorie des modes couplés:

$$i\hbar \cdot \frac{\partial}{\partial t} \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = \begin{pmatrix} \bar{E} & -T \\ -T & \bar{E} \end{pmatrix} \cdot \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix}$$

Deux puits couplés

Théorie des modes couplés:

$$i\hbar \cdot \frac{\partial}{\partial t} \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = \begin{pmatrix} \bar{E} & -T \\ -T & \bar{E} \end{pmatrix} \cdot \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix}$$

«puits de gauche»

«puits de droite»

1) Déterminer les modes globaux normés du système et leurs énergies E_n (fréquences ω_n)

Mode symétrique:

$$E_S = \bar{E} - T$$

$$|\varphi_S\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

Mode anti-symétrique:

$$E_A = \bar{E} + T$$

$$|\varphi_A\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

**2) Projeter le mode d'entrée (au temps t=0) sur ces modes globaux
(produit scalaire entre le mode d'entrée et chaque mode global)**

Input t=0:

$$|\psi^{in}\rangle = \beta_S^{in} |\varphi_S\rangle + \beta_A^{in} |\varphi_A\rangle$$

$$\left. \begin{array}{l} \beta_S^{in} \equiv \langle \varphi_S(x) | \psi^{in}(x) \rangle \\ \beta_A^{in} \equiv \langle \varphi_A(x) | \psi^{in}(x) \rangle \end{array} \right\}$$

**3) Propager chaque mode global dans le temps t>0
avec sa fréquence propre ω_n**

Propagation: $|\psi(t)\rangle = e^{-i\frac{E_S}{\hbar}t} \cdot \beta_S^{in} |\varphi_S\rangle + e^{-i\frac{E_A}{\hbar}t} \cdot \beta_A^{in} |\varphi_A\rangle$

$$|\psi(t)\rangle = e^{-i\frac{E_S+E_A}{2\hbar}t} \cdot \left(e^{-i\frac{\Delta E}{2\hbar}t} \cdot \beta_S^{in} |\varphi_S\rangle + e^{i\frac{\Delta E}{2\hbar}t} \cdot \beta_A^{in} |\varphi_A\rangle \right)$$

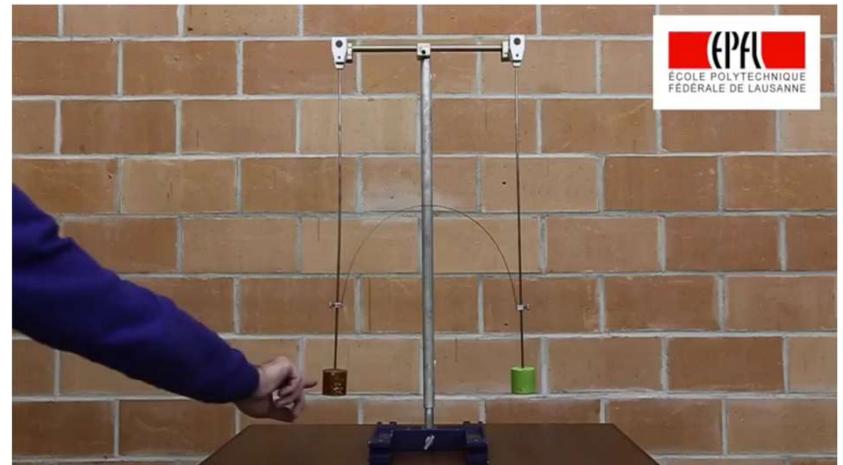
$\Delta E \equiv E_S - E_A = -2T$

Pendules couplés: battements

<https://www.youtube.com/watch?v=aFacOh9hW9U>

Probabilité «Gauche»:

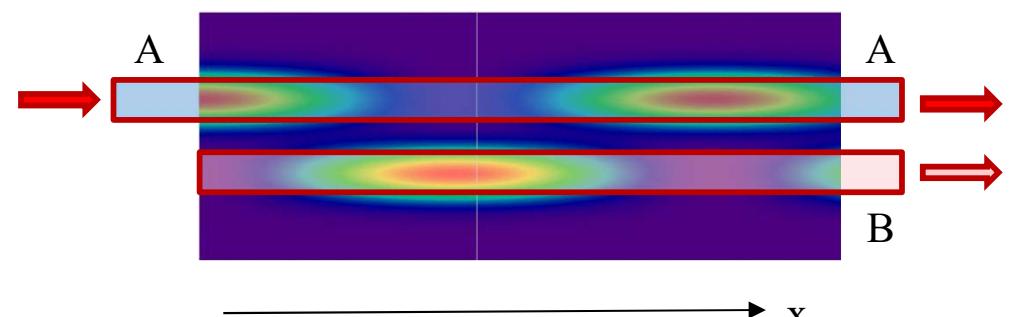
$$P_G(t) = \left| \langle (1, 0) | \psi^{out} \rangle \right|^2 = \cos^2 \left(\frac{\Delta E}{2\hbar} \tau \right)$$



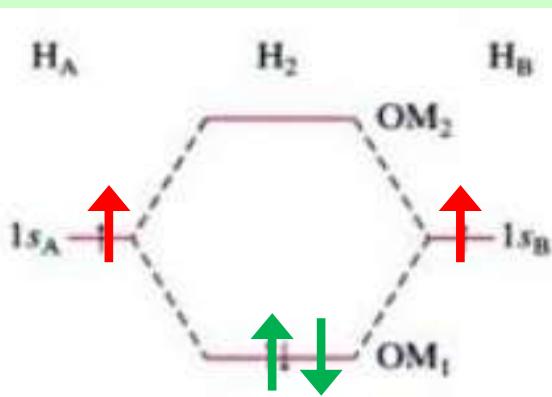
Probabilité «Droite»:

$$P_D(t) = \left| \langle (0, 1) | \psi^{out} \rangle \right|^2 = \sin^2 \left(\frac{\Delta E}{2\hbar} \tau \right)$$

$$\Delta E \equiv E_S - E_A = -2T$$

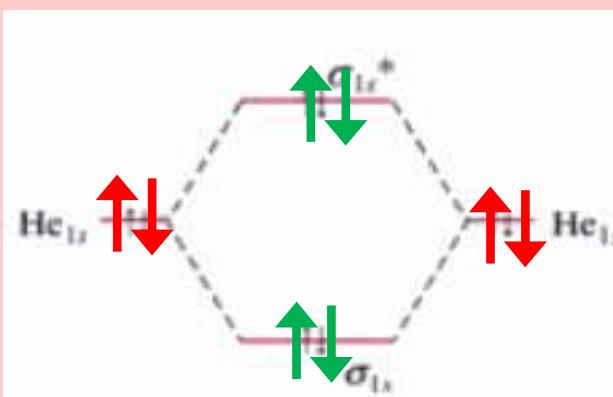


Molécule H₂



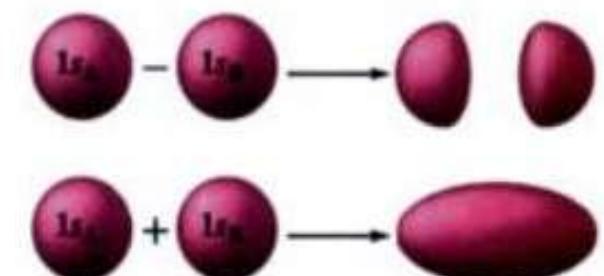
H₂ stable car
énergie plus petite

Molécule He₂



He₂ instable car
énergie égale

Anti-liant



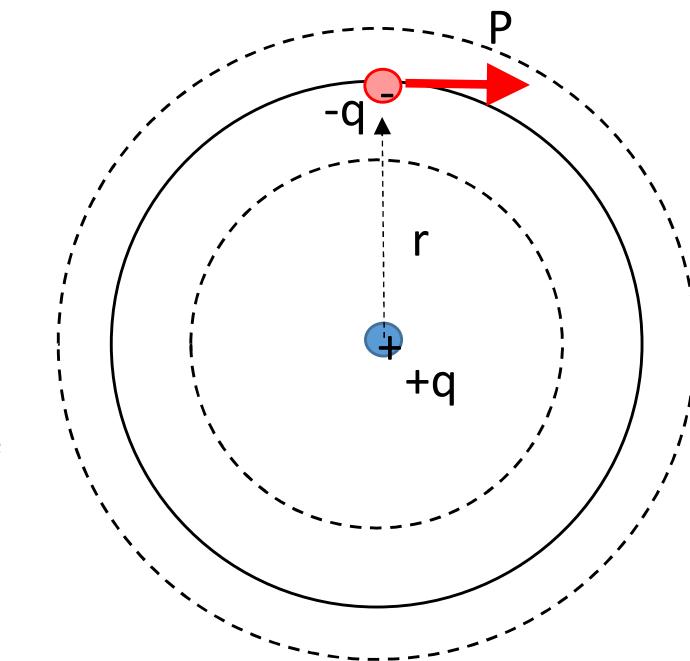
Liant

Exercice 4.1: Atome de Bohr

A) Considérez l'électron comme une **particule classique** et

utilisez le potentiel de Coulomb $E_{pot} = -\left(\frac{q^2}{4\pi\epsilon_0}\right) \cdot \frac{1}{r}$

- 1) Reliez la vitesse et le rayon pour une orbite circulaire stable en équilibrant la force électrique et la force centrifuge.
- 2) Pour ces orbites classiques stables exprimez l'énergie cinétique et l'énergie totale de l'électron en fonction du rayon



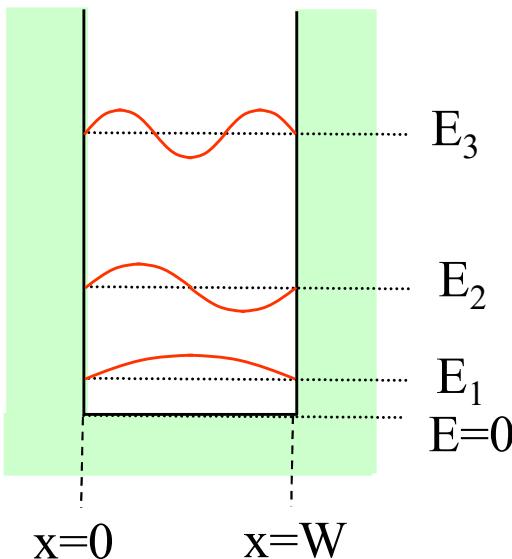
B) Considérez l'électron comme une **onde quantique**

- 3) Reliez le vecteur d'onde au rayon pour une orbite stable
- 4) Exprimez l'énergie cinétique en fonction du rayon

C) Considérez l'électron à la fois comme une **particule classique** et comme une **onde quantique**

- 5) Déterminez l'énergie totale quantifiée.

Exercice 4.3: Evolution temporelle dans un potentiel rectangulaire



Un électron est localisé dans un puit de potentiel rectangulaire de largeur $W=18\text{ um}$ et de profondeur infinie.

Au temps $t=0$, sa fonction d'onde est centrée à $x=W/2$ et elle a la forme:

$$\psi(t=0) \approx e^{-\left(\frac{x-W/2}{a}\right)^2} \quad \text{avec } a = 1\text{ um}$$

Nous définissons le temps caractéristique par $t_c = \frac{\pi \cdot \hbar}{E_2 - E_1}$

$$E_n = \frac{\hbar^2 K^2}{2m} = n^2 \cdot \frac{\hbar^2 \pi^2}{2m W^2}$$

1) Décrivez les étapes nécessaires pour simuler l'évolution temporelle de cet électron.

2) Simulez la fonction d'onde de cet électron aux temps

$$\varphi_n(x) \approx \sin\left(n \cdot \pi \cdot \frac{x}{W}\right)$$

$$t = \frac{1}{N} \cdot \frac{3}{4} t_c \quad \text{avec } N=1, 2, 3, 4 \text{ et } 5$$



Considérez un atome de lithium (Li)
avec trois électrons sur deux niveaux d'énergie.
Dessinez le schéma d'énergie de la cellule Li-Li
contenant deux atomes Li.