MECANIQUE QUANTIQUE

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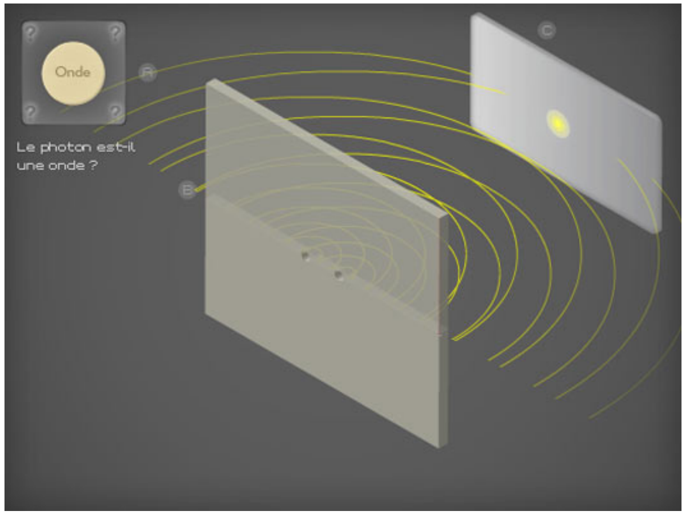
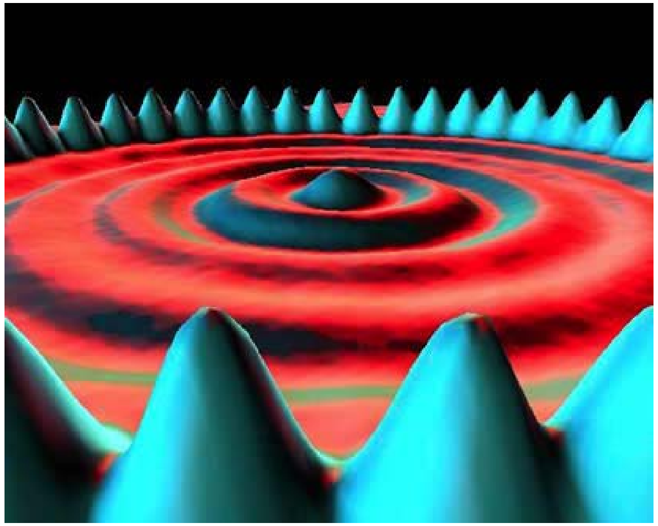
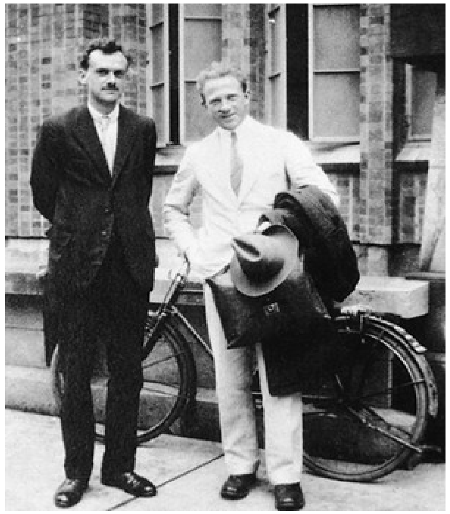






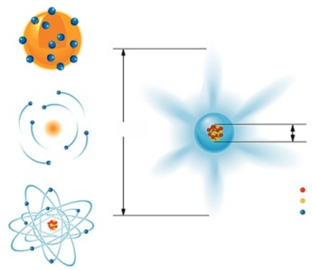
MECANIQUE ONDULATOIRE DE SCHRODINGER

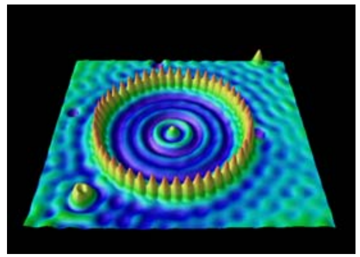
Rappel de cours

1) Dualité onde-corpuscule :

Particule
E, P

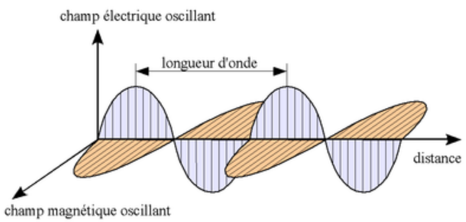
Onde
k, λ, $\omega(\nu)$ tel
E=$\hbar\omega$=hν et λ=h/p ou $\vec{P} = \hbar\vec{k}$
(même que pour un photon)





2) Mvt d'1 particule associé à une onde = Etat d'un système physique = postulat 1

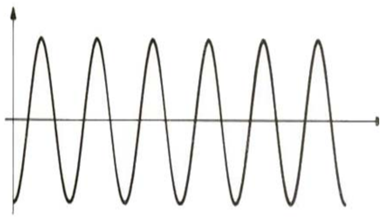
$\Psi(\vec{r},t)$: fonction d'onde



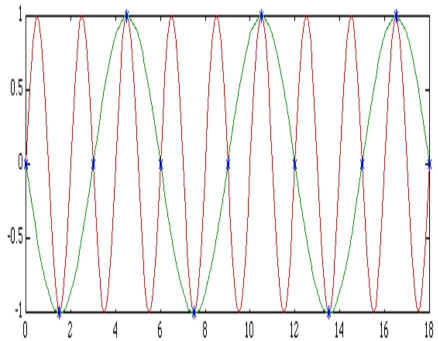
→ Complexe
→ Univoque (r, t→ $\Psi(\vec{r},t)$)
→ Bornée $|\Psi(\vec{r},t)|^2$ est une quantité définie
→ De carré sommable
→ $\Psi(\vec{r},t)$ et $\Psi(\vec{r},t)'$ sont continues car $\Psi(\vec{r},t)''$ intervient dans S
→ $|\Psi(\vec{r},t)|^2 dr = dP$: Probabilité de présence ($\int |\Psi(\vec{r},t)|^2\, dr = 1$)
→ $|\Psi(\vec{r},t)|^2$: Densité de Probabilité de présence

3) Onde plane progressive dans la direction x croissant : $\psi(x,t) = Ae^{i(kx-\omega t)}$

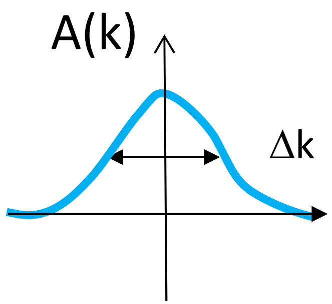
Paquet d'onde : Somme d'ondes planes : $\psi(x,t) = \sum_k A(k)e^{i(kx-\omega t)}$



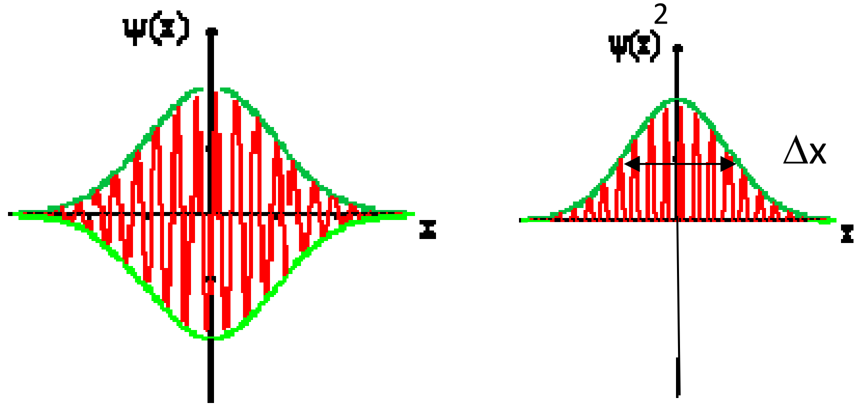
1 OP



2 OP



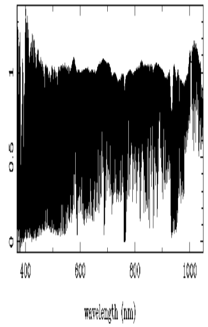
N OP
d'enveloppe
A(k)



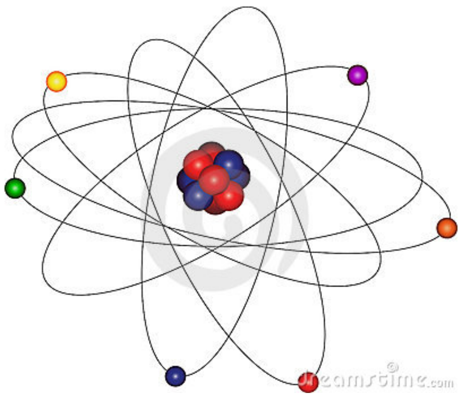
$\Delta x \Delta k \geq \hbar$

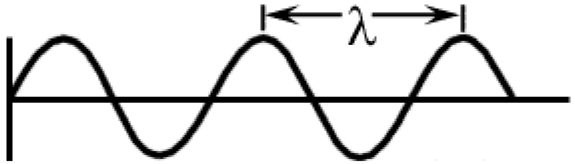
Ordre de grandeur : $\lambda = \frac{h}{p}$

Si objet macroscopique : p ↗ donc λ↘ → on ne voit pas osciller la fonction d'onde



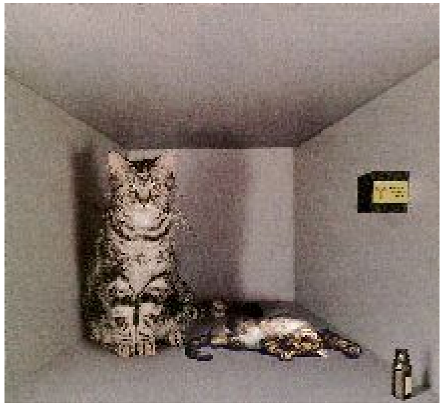
Si objet microscopique : électron p ↘ et λ=12.5Å





4) Postulat 3 : Evolution de $\Psi(\vec{r}, t)$ → EQUATION DE SCHRODINGER dépendant de t

$$\boxed{-\frac{\hbar^2}{2m}\Delta\psi(\vec{r},t) + V(\vec{r},t)\,\psi(\vec{r},t) = i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t}}$$



Energie cinétique   Energie potentielle

A 1D : $[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)]\,\psi(x,t) = i\hbar\frac{\partial}{\partial t}\psi(x,t)$

Quelques exemples

a) Systèmes conservatifs/états stationnaires → Energie totale Ec+Ep=constante

On considère V indép. de t

On cherche des solutions sous la forme $\psi(\vec{r},t)=\varphi(x)f(t)$

$$[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)]\,\varphi(x)f(t) = i\hbar\varphi(x)\frac{df}{dt}$$

$$[-\frac{\hbar^2}{2m}\frac{d^2\varphi(x)}{dx^2}+V(x)\varphi(x)]\,f(t) = i\hbar\varphi(x)\frac{df}{dt}$$

$$[-\frac{\hbar^2}{2m}\frac{d^2\varphi(x)}{dx^2}+V(x)\varphi(x)]/\varphi(x) = i\hbar\frac{df}{f(t)dt} = cst = E$$

$$i\hbar\frac{f'}{f(t)} = E$$

$$\frac{f'}{f(t)} = \frac{E}{i\hbar}dt = -i\frac{E}{\hbar}dt$$

$$\ln\big(f(t)\big) = -i\frac{E}{\hbar}t + C$$

$$f(t) = Ce^{-iEt/\hbar}$$

$$\boxed{\psi(\vec{r},t) = \varphi(x)\,e^{-iEt/\hbar}}$$

Avec $\varphi(x)$ vérifie :

$$[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)]\,\varphi(x) = E\varphi(x)$$

Etats stationnaires ≠ indep. de t mais $|\psi(\vec{r},t)|^2 = |\varphi(x)|^2$

b) Particule libre : V=0

À 1D

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} = i\hbar\frac{\partial\psi(x,t)}{\partial t}$$

$$\boxed{Si\ \psi(x,t) = Ae^{i(kx-\omega t)}} \quad \boxed{\neq\ \psi(x,t) = Ae^{-i(kx-\omega t)}}$$

$$\frac{\partial\psi(x,t)}{\partial t} = -i\omega\psi$$

$$\frac{\partial\psi(x,t)}{\partial x} = ikAe^{i(kx-\omega t)}$$

Et

$$\frac{\partial^2\psi}{\partial x^2} = -k^2\psi$$

$$-\frac{\hbar^2}{2m}(-k^2\psi) = i\hbar(-i\omega\psi)$$

$$\boxed{\frac{\hbar^2k^2}{2m} = \hbar\omega = \frac{p^2}{2m} = E}$$

RESOLUTION DE L'EQUATION DE SCHRODINGER INDEPENDANTE DE t

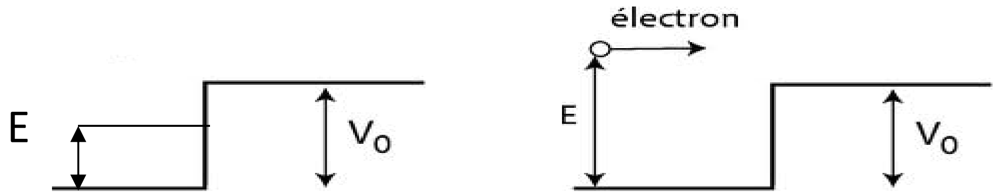
$$-\frac{\hbar^2}{2m}\frac{\partial^2\varphi(x)}{\partial x^2}+V(x)\varphi(x)=E\varphi(x)$$

Ou
$$\frac{\partial^2\varphi(x)}{\partial x^2}+\frac{2m}{\hbar^2}(E-V(x))\varphi(x)=0$$

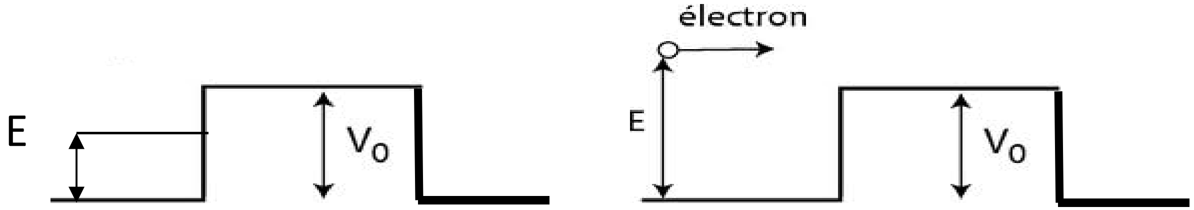
– Equation diff. du second ordre sans terme en $\frac{\partial\varphi(x)}{\partial x}$

- On ne sait la résoudre que si $V = cste$

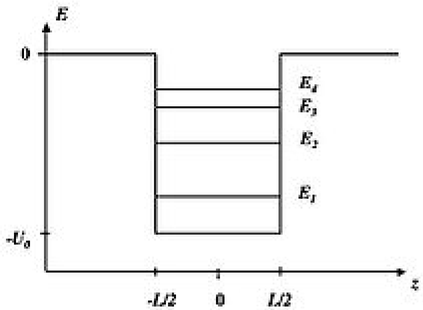
Marche



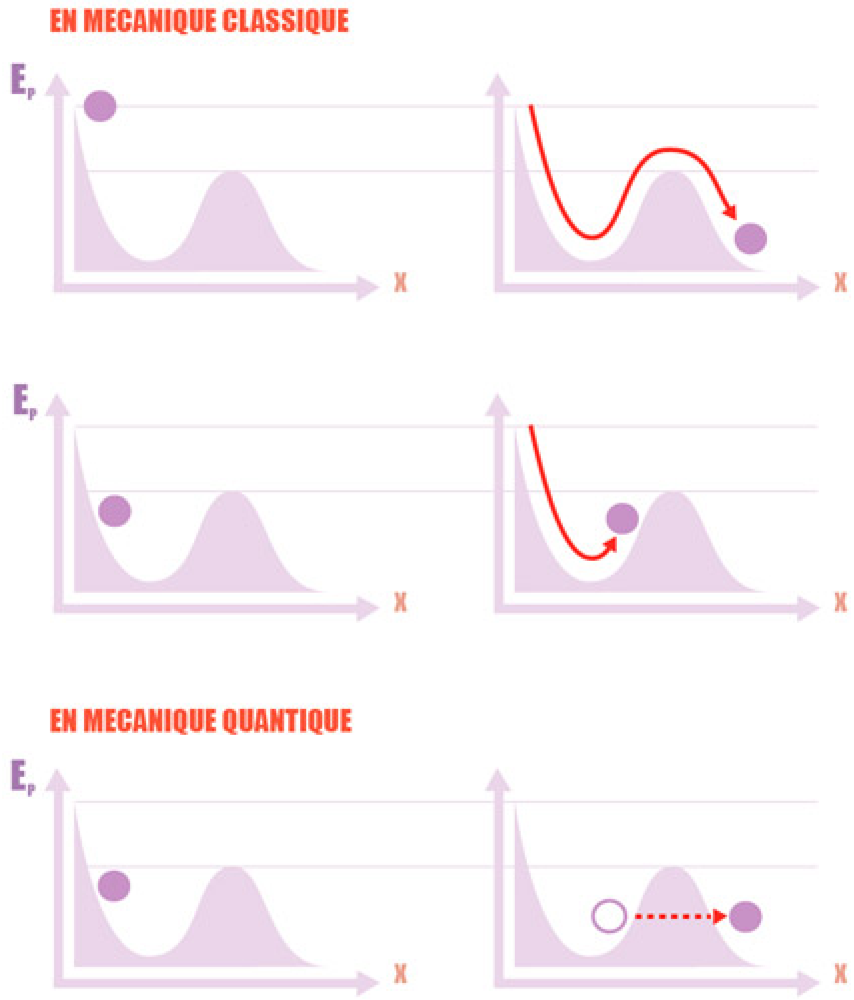
La barrière



Le puits



Comparaison classique / quantique pour la barrière



Que se passe-t-il a une discontinuité de potentiel?

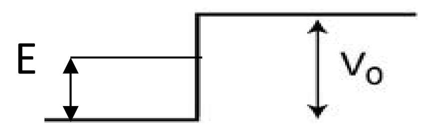
a) Discontinuité finie de potentiel :

$|\psi|^2$ continu → ψ continue

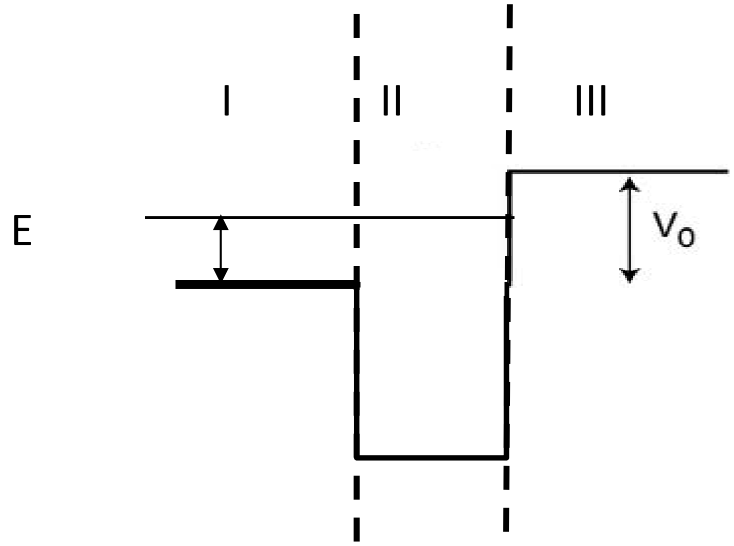
ψ ‘ continue car ψ ‘ ‘ est dans S

b) Discontinuité infinie de potentiel :

ψ (xbord)=0



Résolution de S indépendante de t : Cas général



1) Ecrire équation de S dans chaque région : $-\frac{\hbar^2}{2m}\frac{\partial^2\varphi_i(x)}{\partial x^2}+V(x)\varphi_i(x) = E\varphi_i(x)$

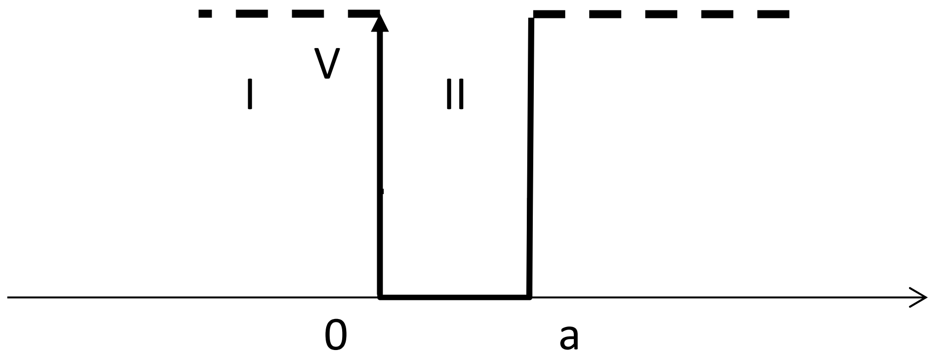
2) Ecrire la solution générale de chaque équation dans chaque région→ on introduit 2 constantes

3) Simplifier les solutions générales = supprimer des constantes = du bon sens

4) Sur chaque discontinuité appliquer les règles précédentes: conditions aux limites

Puits de potentiel carré infini

Pour $0<x<a$ $V(x)=0$



$$1)\quad -\frac{\hbar^2}{2m}\frac{\partial^2\varphi(x)}{\partial x^2} = E\varphi(x)$$

2) Solution générale : $\varphi(x) = A\sin(kx+\eta)$ $\qquad$ $(2\ constantes\ A\ et \eta)$

3) Conditions aux limites : $\varphi(x=0) = \varphi(x=a) = 0$ $\qquad$ $(\varphi(x<0)$=0=$\varphi(x>a))$

$\varphi(x=0) \rightarrow \eta = 0$ $\quad$ et $\quad$ $\varphi(x=a)$= $A\sin(ka) = 0 \rightarrow$ *ka=nπ*

$\varphi(x) = A\sin(kx)$ avec $k_n = \frac{n\pi}{a}$

Or $k_n{}^2 = \frac{2mE_n}{\hbar^2}$

$$\boxed{\rightarrow E_n = \frac{\hbar^2 k_n{}^2}{2m} = n^2\frac{\hbar^2\pi^2}{2ma^2}}$$

Puits de potentiel carré infini : Solutions ($E_n = \frac{\hbar^2 {k_n}^2}{2m} = n^2 \frac{\hbar^2 \pi^2}{2ma^2}$)

Niveau fondamental : n=1

$$E_1 = \frac{\hbar^2 \pi^2}{2ma^2}$$

$$\varphi(x) = A \sin(\frac{\pi}{a} x)$$

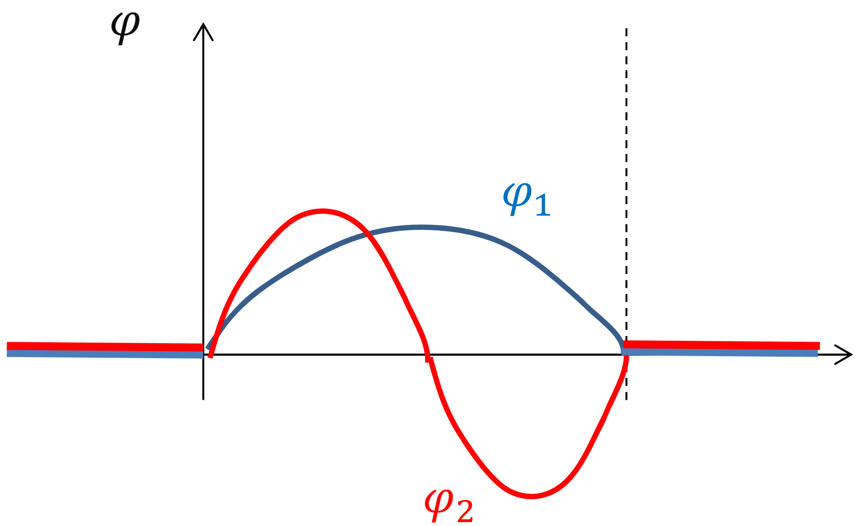
a=10^{-10}m → $E_1 = \frac{\pi^2 (1{,}054.10^{-34})^2}{2*0{,}9*10^{-30}*10^{-20}*1{,}6*10^{-19}} = 38eV$

Premier niveau excité : n=2

$$E_2 = \frac{4\hbar^2 \pi^2}{2ma^2} = 4E_1$$

$$\varphi(x) = A \sin(\frac{2\pi}{a} x)$$

$$E_2 = 152\ eV$$



Puits de potentiel carré infini : Solutions

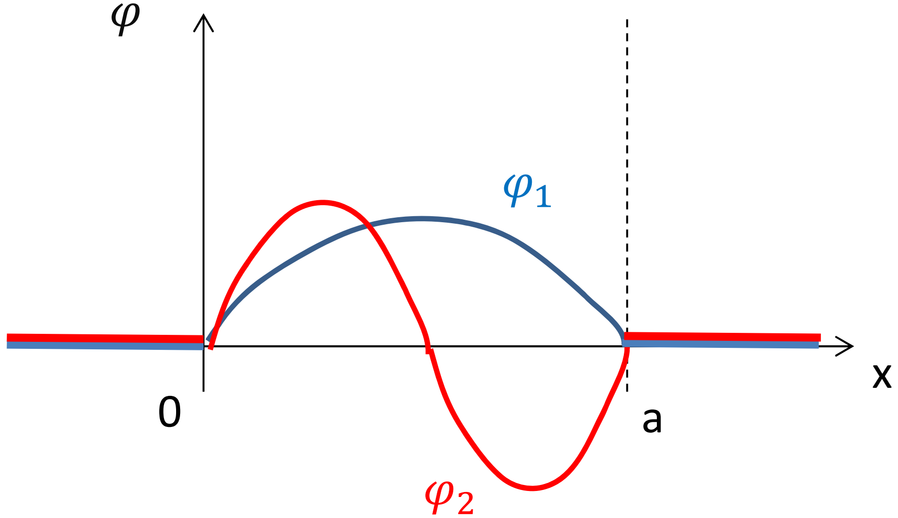
$$P_{0\to a} = \int_{-\infty}^{\infty} |\varphi_2(x)|^2\, dx = 1$$

$$P_{0\to a} = 1 = \int_0^a |\varphi_1(x)|^2\, dx = \int_0^a |A|^2 \sin^2\frac{\pi x}{a}\, dx = 1 = |A|^2 \int_0^a \frac{1 - \cos\frac{2\pi x}{a}}{2}\, dx = |A|^2 \frac{a}{2}$$

$$\rightarrow |A| = \sqrt{\frac{2}{a}}$$

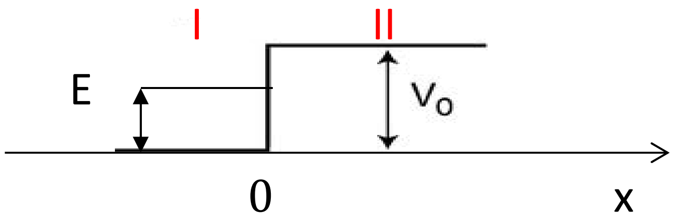
$$P_{0\to a/2} = \int_0^{a/2} |\varphi_2(x)|^2\, dx = \frac{2}{a}\int_0^{a/2} \sin^2\frac{2\pi x}{a}\, dx = \frac{2}{a}\int_0^{a/2} \frac{1 - \cos\frac{4\pi x}{a}}{2}\, dx = \frac{1}{2}$$

Comme intuité au regard de la courbe



La marche de potentiel à 1D

Marche



$E>V_0$ → seul cas en méca classique

<u>Description classique</u> :

Car $\frac{p^2}{2m} = E$ ou $\frac{p^2}{2m} = E - V_0$

1 onde incidente et 1 transmise : $v_I = \sqrt{\frac{2E}{m}}$ et $v_{II} = \sqrt{\frac{2(E-V_0)}{m}}$

<u>Description quantique</u> : réflexion partielle+transmission

Région I : $k^2_I = \frac{2mE}{\hbar^2}$

$$\frac{\partial^2\varphi_I(x)}{\partial x^2} + \frac{2mE}{\hbar^2}\varphi_I(x) = 0$$

$$\varphi_I = Ae^{ik_Ix} + Be^{-ik_Ix}$$

Région II : $k_{II^2} = \frac{2m(E-V_0)}{\hbar^2}$

$$\frac{\partial^2\varphi II(x)}{\partial x^2} + \frac{2m(E-V_0)}{\hbar^2}\varphi_{II}(x) = 0$$

$$\varphi_{II} = Ce^{ik_{II}x} + \cancel{De^{-ik_{II}x}}$$

La marche de potentiel à 1D

$$\varphi_I = Ae^{ik_Ix} + Be^{-ik_Ix}$$

$$\varphi_{II} = Ce^{ik_{II}x} + \cancel{De^{-ik_{II}x}}$$

$$\left\{\begin{array}{l} A+B=C \quad \varphi \text{ continu} \\ ik_I(A-B) = ik_{II}C \quad \varphi' \text{ continu} \end{array}\right.$$

$$1 + \frac{B}{A} = \frac{C}{A}$$

$$1 - \frac{B}{A} = \frac{k_{II}}{k_I}\frac{C}{A}$$

$$2 = \frac{C}{A}\left(1 + \frac{k_{II}}{k_I}\right)$$

$$\frac{C}{A} = \frac{2}{1+\frac{k_{II}}{k_I}} \quad \rightarrow \boxed{R = \left|\frac{B}{A}\right|^2}$$

$$\frac{B}{A} = \frac{C}{A} - 1 = \frac{2}{1+\frac{k_{II}}{k_I}} - 1 = \frac{2-1-\frac{k_{II}}{k_I}}{1+\frac{k_{II}}{k_I}} = \frac{1-\frac{k_{II}}{k_I}}{1+\frac{k_{II}}{k_I}} = \frac{k_I-k_{II}}{k_I+k_{II}}$$

$$\frac{B}{A} = \frac{k_I-k_{II}}{k_I+k_{II}} \quad \rightarrow \boxed{T = 1-R = 1-\left(\frac{k_I-k_{II}}{k_I+k_{II}}\right)^2 = \frac{4k_Ik_{II}}{(k_I+k_{II})^2} = \left|\frac{C}{A}\right|^2 \frac{k_{II}}{k_I}}$$

La marche de potentiel à 1D :
Cas physique de la surface d'un matériaux pour un électron libre

$E<V_0 \rightarrow E-V_0<0$

<u>Description quantique seule possible</u> : Transmission possible

Région I : $k_I = \sqrt{\frac{2mE}{\hbar^2}}$

$$\frac{\partial^2 \varphi I(x)}{\partial x^2} + \frac{2mE}{\hbar^2}\, \varphi_I(x) = 0$$

$$\varphi_I = Ae^{ikx} + Be^{-ikx}$$

Région II : $k_{II} = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$

$$\frac{\partial^2 \varphi II(x)}{\partial x^2} + \frac{2m(E-V_0)}{\hbar^2}\, \varphi_{II}(x) = 0$$

$$\varphi_{II} = Ce^{-K_{II}x} + \cancel{De^{K_{II}x}}$$

$$\varphi_I(0) = \varphi_{II}(0)$$

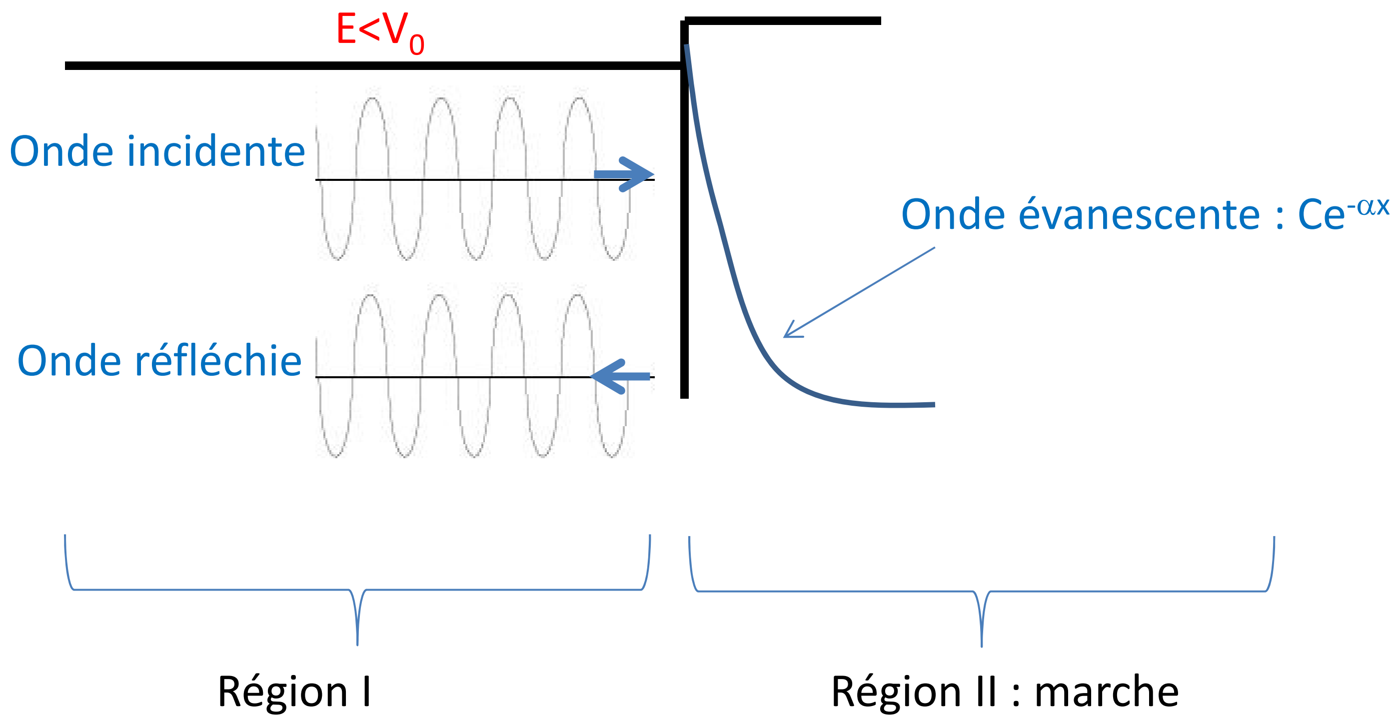
$$\varphi'_I(0) = \varphi'_{II}(0)$$

$$\left.\begin{array}{l} A+B=C \\ ik(A-B) = -\alpha C \end{array}\right\}$$

$$\left.\begin{array}{l} 1 + \frac{B}{A} = \frac{C}{A} \\ ik\left(1 - \frac{B}{A}\right) = -\alpha \frac{C}{A} \end{array}\right\}$$

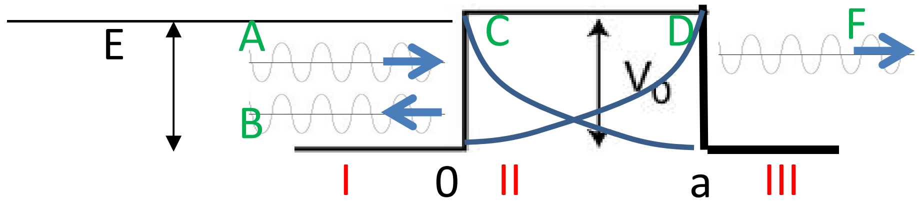
$$ik\left(2 - \frac{C}{A}\right) = -\alpha \frac{C}{A} \rightarrow \frac{C}{A}(ik-\alpha) = 2ik$$

$$\frac{C}{A} = \frac{2k}{k+i\alpha} \quad \text{et} \quad \frac{B}{A} = \frac{k-i\alpha}{k+i\alpha} \qquad \boxed{R = \left|\frac{B}{A}\right|^2 = 1} \quad \rightarrow \quad R+T=1 \rightarrow \boxed{T=0}$$



Même chose avec une barrière finie de potentiel
→ Effet tunel

Facteur de transmission d'une barrière de potentiel : Application au microscope à effet tunnel ou STM



$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

$$K^2 = \frac{2m(-E+V_0)}{\hbar^2}$$

1) Région I : $\frac{\partial^2 \varphi_I(x)}{\partial x^2} + \frac{2mE}{\hbar^2}\varphi_I(x) = 0$

$$\varphi_I = Ae^{ikx} + Be^{-ikx}$$

$$\varphi'_I = ik(Ae^{ikx} - Be^{-ikx})$$

Région II : $\frac{\partial^2 \varphi_{II}(x)}{\partial x^2} + \frac{2m(E-V_0)}{\hbar^2}\varphi_{II}(x) = 0$

$$\varphi_{II} = Ce^{-Kx} + De^{Kx}$$

$$\varphi'_{II} = K(De^{Kx} - Ce^{-Kx})$$

Région III : $\frac{\partial^2 \varphi_{III}(x)}{\partial x^2} + \frac{2mE}{\hbar^2}\varphi_{III}(x) = 0$

$$\varphi_{III} = Fe^{ikx} + Ge^{-ikx}$$

$$\varphi'_{III} = ikFe^{ikx}$$

On pose A=1 et la Continuité de φ et φ'

1+B=C+D

ik(1-B)=K(D-C)

$$Fe^{ika} = Ce^{-Ka} + De^{Ka}$$

$$K(De^{Ka} - Ce^{-Ka}) = ikFe^{ika}$$

$$\Rightarrow \left\{ \begin{array}{l} 1+B=C+D \\ 1 - B = i\frac{K}{k}(C-D) \\ Fe^{ika} = Ce^{-Ka} + De^{Ka} \\ -Fe^{ika}\frac{ik}{K} = Ce^{-Ka} - De^{Ka} \end{array} \right.$$

$$\boxed{\begin{array}{l} 1+B=C+D \\ 1-B = i\dfrac{K}{k}(C-D) \\ Fe^{ika} = Ce^{-Ka} + De^{Ka} \\ -Fe^{ika}\dfrac{ik}{K} = Ce^{-Ka} - De^{Ka} \end{array}}$$

3) ka<<1 Barrière infiniment mince

e^{Ka} =1 et $e^{ika} = 1$

$$\left\{\begin{array}{l} 1+B=C+D \\ ik(1-B) = K(D-C) \\ F = C + D(= 1 + B) \\ K(D-C) = ikF \end{array}\right. \Rightarrow \left\{\begin{array}{l} (1-B) = F \\ (1+B) = F \end{array}\right. \Rightarrow \left\{\begin{array}{l} 2 = 2\mathrm{F} \rightarrow F = 1 \text{ et B=0 car A=1} \\ \text{La barrière n'existe pas} \\ \qquad\qquad \text{T=1 : transmission totale} \end{array}\right.$$

4) ka>>1 Barrière infiniment épaisse (ou $K^2 = \frac{2m(-E+V_0)}{\hbar^2}$ → soit K↗ V_0-E↗ : marche haute ou m ↗ particule lourde)

$e^{Ka} \gg 1$ et D<<C

$$1+B=C$$

$$ik(1-B) = -KC$$

$$(1-B) = -\frac{K}{ik}C = i\frac{K}{k}C$$

$$2 = C\left(1 + i\frac{K}{k}\right)$$

$$\rightarrow C = \frac{2}{1+i\frac{K}{k}}$$

$$k^2 + K^2 = \frac{2mE}{\hbar^2} + \frac{2m(V_0 - E)}{\hbar^2} = \frac{2mV_0}{\hbar^2}$$

$$k^2 K^2 = \frac{2m(V_0 - E)}{\hbar^2}\frac{2mE}{\hbar^2} = +\frac{4m^2 E(V_0 - E)}{\hbar^4}$$

$$|F|^2 = \frac{16\frac{4m^2 E(V_0 - E)}{\hbar^4} e^{-2Ka}}{\frac{4m^2 V_0^2}{\hbar^4}} = \frac{16E(V_0 - E)e^{-2Ka}}{V_0^2} = \mathrm{T}$$

5) $\mathrm{T} = \dfrac{4E(V_0 - E)}{4E(V_0 - E) + V_0^2 sh^2 Ka}$

Ka<<1 shKa= $\dfrac{e^{Ka} - e^{-Ka}}{2}$

$$e^{Ka} \approx e^{-Ka} = 1 \rightarrow shka = 0 \rightarrow \mathrm{T(E)} \approx 1$$

Ka>>1 shKa= $\dfrac{e^{Ka} - e^{-Ka}}{2} \approx \dfrac{e^{Ka}}{2}$

$$\mathrm{T} = \frac{4E(V_0 - E)}{4E(V_0 - E) + V_0^2 sh^2 Ka} = \frac{4E(V_0 - E)}{4E(V_0 - E) + V_0^2 \frac{e^{2Ka}}{4}} \sim \frac{16E(V_0 - E)e^{-2Ka}}{V_0^2}$$

V_0=2eV et $E_0 = 1eV$ T=$\sim \frac{16E(V_0-E)e^{-2Ka}}{{V_0}^2}$

T= $\frac{16*1*1*e^{-2Ka}}{4}$

K= $\sqrt{\frac{2*9*10^{-31}(2-1)*1{,}6*10^{-19}}{(1.054*10^{-24})^2}} = 5.0888 * 10^9$

T=$\frac{16}{4}e^{-2*2{,}54} = 0{,}0246$=2,46%

Ka=$5.0888 * 10^9$*5*$10^{-10} = 2{,}54 \gg 1!$

$\frac{\Delta T}{T} = -2K\Delta a$ $\Delta a = \frac{\Delta T}{T}\frac{1}{(-2K)} = -0{,}1\frac{1}{-2*5{,}09*10^9} = 9.8 * 10^{-12}m \approx 0{,}1Å$

Calcul sans approx :

T=$\frac{4*1*4}{4*1*1+4sh^2 2.54} = 0{,}0245$ =2,45%

→ APPLICATION MICROSCOPE a EFFET TUNEL