Lezione Speciale 28/03/2017

Approssimazione semi-classica (WKB approximation)

(Wentzel-Kramers-Brillouin)

- Il limite semiclassico della MQ
- Sviluppo in $\hbar$: funzione d'onda semi-classica
- Formula di connessione
- Applicazione 1: stati legati e quantizzazione di Bohr-Sommerfeld
- Applicazione 2: effetto tunnel.

- Il limite semiclassica della MQ

Eq. di Schrödinger:

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r}) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi(\mathbf{r}) \qquad (*)$$

Il limite $\hbar \longrightarrow 0$ non può essere preso in maniera naïva.

Un hint: particella libera ~ $e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}$ $\quad \lambda = h/p \longrightarrow 0$

In generale: $\psi \sim e^{iS/\hbar}, \qquad S \sim O(\hbar^0)$ $\quad (**)$

Sostituendo $\psi = A\, e^{iS/\hbar}$ in (*) si ha

$$\hbar^0 \quad : \quad \frac{\partial}{\partial t}S = -\frac{1}{2m}(\nabla S)^2 - V$$

Equazione di Hamilton-Jacobi

$$\hbar^1 \quad : \quad \frac{\partial}{\partial t}(A^2) + \nabla(A^2\frac{\nabla S}{m}) = 0$$

Equazione di continuità

$$A^2 = |\psi|^2 = \rho, \qquad \frac{\nabla S}{m} = \frac{\mathbf{p}}{m} = \mathbf{v}$$

$$S = \int dt\, L = \int dt\{\sum_i p_i\dot{q}_i - H\} = \sum_i \int^q dq_i p_i - \int^t dt H$$

Funzione principale di Hamilton (l'azione classica)

$$\partial S/dq_i = p_i, \qquad -\partial S/dt = H$$

Quindi: S= l'azione classica!

Funzione d'onda semi-classica (Sviluppo in $\hbar$)

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

$$\psi(x) = \exp\left(i\frac{\sigma}{\hbar}\right) ,$$

$$\sigma(x) = \sum_{k=0}^{\infty}\left(\frac{\hbar}{i}\right)^k \sigma_k = \sigma_0 + \frac{\hbar}{i}\,\sigma_1 + \left(\frac{\hbar}{i}\right)^2 \sigma_2 + \dots \,. \qquad \Rightarrow$$

$$(\sigma')^2 - i\,\hbar\,\sigma'' = p^2(x)\,, \qquad p^2(x) = 2\,m\,\left(E - V(x)\right)\,,$$ (impulso classico)

$$\Rightarrow \qquad (\sigma_0')^2 = p^2\,;\ \sigma_0 = \pm\int p(x)dx\,;\ p(x) = +\sqrt{2\,m\,(E - V(x))}\,.$$ (*)

$$\sigma_1' = -\frac{1}{2\sigma_0'}\sigma_0'' \quad \Rightarrow \quad \sigma_1 = -\frac{1}{2}\log(p)\,;$$

$$\sigma_n' = -\frac{1}{2\sigma_0'}\left(\sum_{k=1}^{n-1}\sigma_k'\sigma_{n-k}' + \sigma_{n-1}''\right)\,; \qquad n \geq 2\,.$$

$$\Rightarrow \qquad e^{i\,\frac{\sigma}{\hbar}} \simeq \frac{1}{\sqrt{p(x)}}\exp\left(i\int_{x_0}^{x}\left[\frac{1}{\hbar}\,p(x)\right]\,dx\right)\,;$$ $\hbar^0 \qquad \hbar^1$

Ma in (*) p prende i segni +/-, E <V o E>V ⇒

$$\psi(x) = b_1 \frac{1}{\sqrt{p}} e^{\frac{i}{\hbar}\int_{x_0}^{x} p(x)\,dx} + b_2 \frac{1}{\sqrt{p}} e^{-\frac{i}{\hbar}\int_{x_0}^{x} p(x)\,dx} ;$$

N.B. onde piane per V=cost.

- p(x) reale (E> V): nelle regioni classicamente accessibile;
- p(x) immaginario (p(x) → i |p(x)|) (E < V): nelle regioni classicamente inaccessibile;

Ma l'approssimazione semiclassica

$$(\sigma')^2 - i\,\hbar\,\sigma'' = p^2(x)\,,$$ richiede che

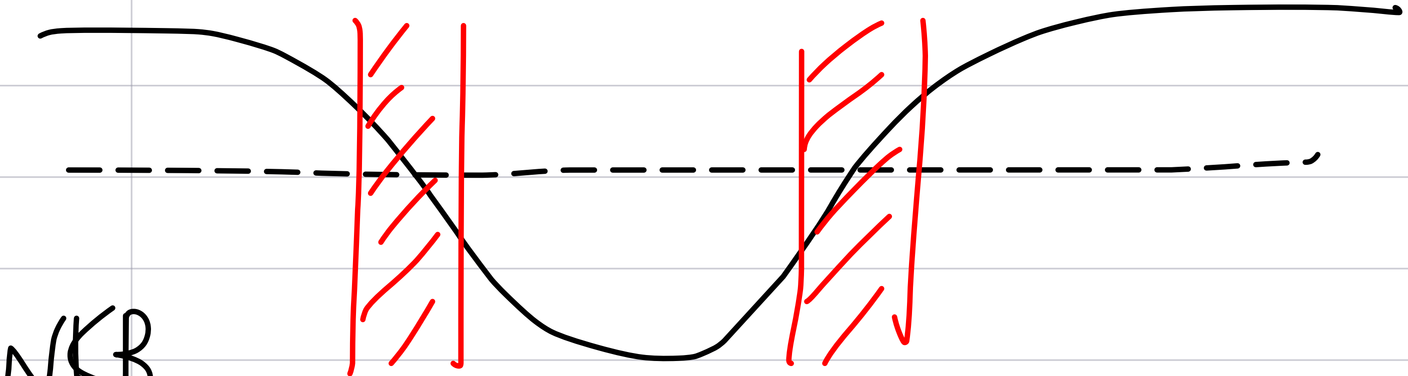
$$\hbar|\sigma''| \ll (\sigma')^2$$ - - - - - - - - - - - - →

$$\frac{1}{2}\,\hbar\frac{p'}{p^2} \ll 1 \quad \Rightarrow \quad \frac{1}{4\pi}\,\frac{d\lambda}{dx} \ll 1\,; \qquad \lambda = \frac{h}{p}\,;$$

∴ l'approssimazione non è valida vicino ai punti di ritorno classici (p=0).

Q:

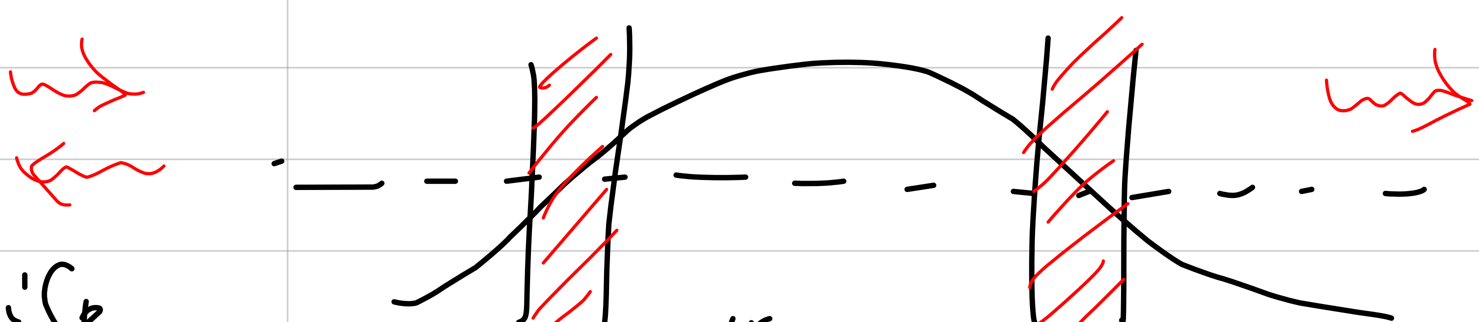
Come trovare la connessione tra la funzione d'onda valida a E>V e quella a E<V, attraveso la regione dove l'approssimazione fallisce ???



WKB ok — NO — WKB ok — NO — WKB ok

$$\frac{B}{\sqrt{|p|}} e^{\frac{1}{\hbar}\int^x |p| dx} \qquad \frac{1}{\sqrt{p}} A e^{\frac{i}{\hbar}\int^x p} + \frac{A'}{\sqrt{p}} e^{-\frac{i}{\hbar}\int^x p} \qquad \frac{C}{\sqrt{|p|}} e^{-\frac{1}{\hbar}\int^x |p| dx}$$

⇒ **FORMULE DI CONNESSIONE**



$$e^{\frac{i}{\hbar}\int p} + B e^{-\frac{i}{\hbar}\int p} \qquad A e^{-\frac{1}{\hbar}\int |p|} + A' e^{\frac{1}{\hbar}\int |p| dx} \qquad C \cdot e^{\frac{i}{\hbar}\int dx\, p}$$

IDEA!!!

Attorno ad un punto di ritorno classico (p(x) ~ 0, x~ a)

- Utilizzare l'approssimazione lineare invece: i.e.,

  E-V(x) = c. (x-a) = c z

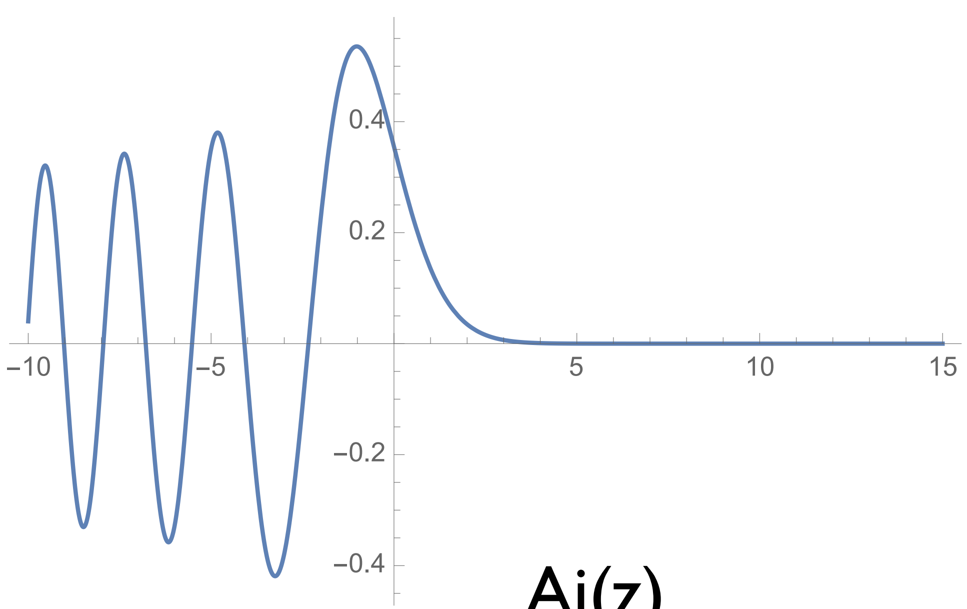
- Risolvere esattamente l'eq. di Schroedinger;

$$-\frac{\hbar^2}{2m}\psi'' = (E - V(x))\psi \qquad\qquad \psi'' + \beta^2(a - x)\psi = 0$$

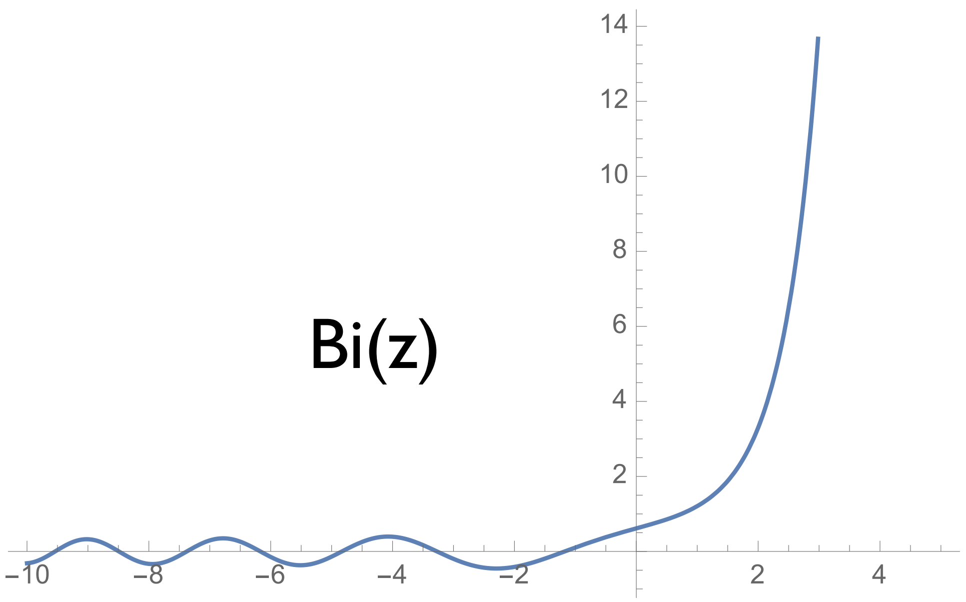
$$d^2\psi/dz^2 - z\psi = 0\;; \qquad (x - a = \beta^{-2/3}\, z)\;;$$

Campo elettrico costante in 1D

Le soluzioni sono le funzioni di Airy, Ai(z) e Bi(z)



Ai(z)



Bi(z)

(*) Approssimazione lineare

$E - V(x) = c.\,(x-a)$
$= c\, z$

$$c_1 \frac{1}{\sqrt{p}} e^{\frac{i}{\hbar}\int p\,dx} + c_2 \frac{1}{\sqrt{p}} e^{-\frac{i}{\hbar}\int p\,dx} \quad \Downarrow \quad \psi^{(1)}(z) = A_i(z) \qquad \psi^{(2)}(z) = B_i(z) \qquad c_1' \frac{1}{\sqrt{|p|}} e^{-\frac{1}{\hbar}\int |p|} + c_2' \frac{1}{\sqrt{|p|}} e^{\frac{1}{\hbar}\int |p|}$$

La relazione $(c_1, c_2) \Longleftrightarrow (c_1', c_2')$ possono essere determinati dalla regioni di compatibilità (zone verdi)

Ai, Bi = Airy functions

- Raccordare l'andamento asintotico della soluzione centrale x ~a

$$\frac{|z|^{-\frac{1}{4}}}{\sqrt{\pi}}\cos\left(\frac{2}{3}|z|^{3/2}-\frac{\pi}{4}\right) \underset{z\to-\infty}{\longleftarrow} \mathrm{Ai}(z) \underset{z\to\infty}{\longrightarrow} \frac{1}{\sqrt{\pi}}\frac{1}{2}z^{-1/4}e^{-\frac{2}{3}|z|^{3/2}}\;; \tag{11.12a}$$

$$-\frac{|z|^{-\frac{1}{4}}}{\sqrt{\pi}}\sin\left(\frac{2}{3}|z|^{3/2}-\frac{\pi}{4}\right) \underset{z\to-\infty}{\longleftarrow} \mathrm{Bi}(z) \underset{z\to\infty}{\longrightarrow} \frac{1}{\sqrt{\pi}}z^{-\frac{1}{4}}e^{+\frac{2}{3}|z|^{3/2}}\,. \tag{11.12b}$$

con le soluzioni WKB a |x-a| piccolo, con

$$p=\hbar\,\beta(a-x)^{\frac{1}{2}}=\hbar\,\beta^{\frac{1}{3}}\sqrt{-z}\;;\quad w(a,x)=-\frac{2}{3}\beta(a-x)^{\frac{3}{2}}=-\frac{2}{3}|z|^{\frac{3}{2}}\;;$$

$$\tilde{p}=\hbar\,\beta(x-a)^{\frac{1}{2}}=\hbar\,\beta^{\frac{1}{3}}\sqrt{z}\;;\quad \tilde{w}(a,x)=\frac{2}{3}\beta(x-a)^{\frac{3}{2}}=\frac{2}{3}|z|^{\frac{3}{2}}\,.$$

From eqn (11.12) it follows that the two independent solutions are

$$\frac{1}{\sqrt{p}}\cos\left(|w(a,x)|-\frac{\pi}{4}\right) \underset{x\to-\infty}{\longleftarrow} \psi \underset{x\to\infty}{\longrightarrow} \frac{1}{2}\frac{1}{\sqrt{\tilde{p}}}e^{-|\tilde{w}|}\;; \tag{11.13a}$$

$$-\frac{1}{\sqrt{p}}\sin\left(|w(a,x)|-\frac{\pi}{4}\right) \underset{x\to-\infty}{\longleftarrow} \psi \underset{x\to\infty}{\longrightarrow} \frac{1}{\sqrt{\tilde{p}}}e^{+|\tilde{w}|}\,. \tag{11.13b}$$

$$w(a,x) = \frac{1}{\hbar}\int_a^x p(x)dx\ , \qquad p(x) = \sqrt{2m(E - V(x))}$$

$$\tilde{w}(a,x) = \frac{1}{\hbar}\int_a^x |p(x)|dx\ , \qquad |p(x)| = \sqrt{2m(V(x) - E)}$$

Quantizzazione di Bohr-Sommerfeld

Stati legati

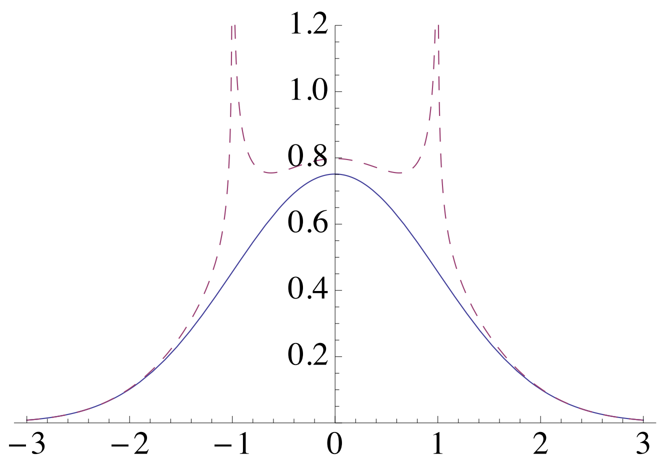
$$\oint dq\, p = 2\pi\hbar\,(n + \frac{1}{2}) = h\,(n + \frac{1}{2})$$

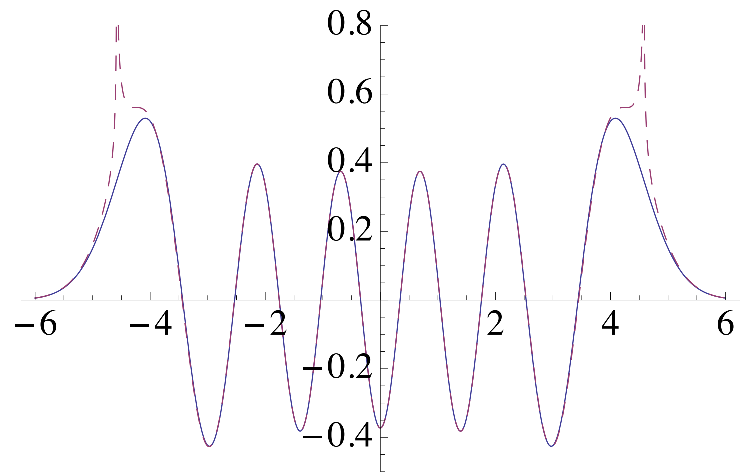
(*)

cfr. Bohr-Sommerfeld originale

Osservazioni:

- Ogni stato quantistico "occupa" il volume $\Delta q \Delta p \sim 2\pi\hbar$
- per Oscilatore armonico il risultato è esatto! Ma w.f. ?





- (*) OK per n >>1: molte oscillazioni, λ ben definita
- per Oscilatore quartico $p = \sqrt{2m(E - \frac{g}{2}x^4)}$

The quartic potential

A less trivial case concerns the quartic potential, $U = \frac{g}{2}x^4$:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}\,gx^4\psi = E\psi\,. \tag{11.45}$$

By making a transformation $x = \lambda z$, with $\lambda = (\hbar^2/mg)^{1/6}$ we see that eqn (11.45) transforms into

$$-\frac{1}{2}\frac{d^2\psi}{dz^2} + \frac{1}{2}z^4\psi = \frac{\epsilon}{2}\psi\,; \qquad \frac{\epsilon}{2} = E\left(\frac{m}{\hbar^2}\right)^{2/3} g^{-1/3}\,. \tag{11.46}$$

The eigenvalues of eqn (11.46) do not depend on any parameter, and hence it suffices to study it and put at the end

$$E_n = \left(\frac{\hbar^2}{m}\right)^{2/3} g^{1/3}\,\frac{\epsilon}{2}\,. \tag{11.47}$$

For eqn (11.46) the turning points are $z = \pm a = \pm\varepsilon^{1/4}$ and the quantization condition can be written as[5]

$$n + \frac{1}{2} = \frac{1}{2\pi}\sqrt{\varepsilon}\,2\int_{-a}^{a}\sqrt{1-\left(\frac{z}{a}\right)^4}\,dx = \frac{2}{\pi}a\,\sqrt{\varepsilon}\,I\,,$$

$$I = \frac{1}{4}\,B\left(\tfrac{1}{4},\tfrac{3}{2}\right) = \frac{\sqrt{\pi}\,\Gamma\left(\frac{1}{4}\right)}{8\,\Gamma\left(\frac{7}{4}\right)} = 0.874\,019\,2\ldots\,,$$

from which

$$\varepsilon_n = \left[\frac{\pi}{2I}(n+\frac{1}{2})\right]^{4/3}\,.$$

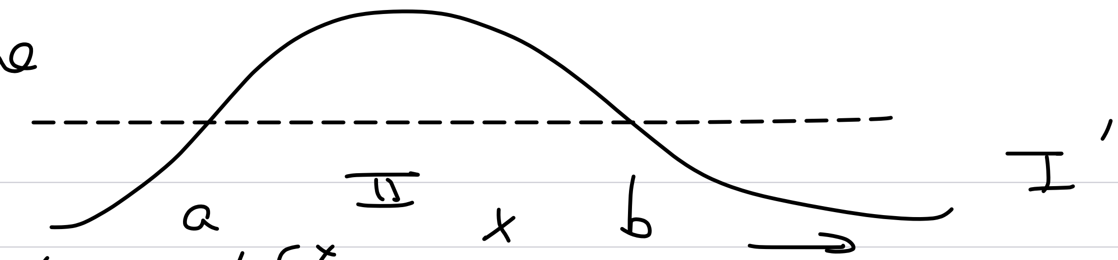
A comparison between the WKB results here and the exact levels (which can be found by the variational method discussed in the previous chapter) is shown below:

n	ε_n	ε_n^{WKB}	$\delta\varepsilon/\varepsilon$
0	1.060 36	0.867 15	0.182 22
1	3.799 67	3.751 92	0.012 57
2	7.455 70	7.413 99	0.005 59
3	11.644 75	11.611 53	0.002 85
4	16.261 83	16.233 61	0.001 73
5	21.238 37	21.213 65	0.001 16

[5] $B(p,q)$ is Euler's beta function.

Effetto Tunnel

Diffusione



$$x \to \infty \quad \psi^{(I')} \sim \frac{1}{\sqrt{p}} e^{\frac{i}{\hbar}\int_b^x dx\, p(x)} = \psi^{(1)} - i\,\psi^{(2)} \quad (\bullet)$$

$$= \frac{C}{\sqrt{p}}\, e^{\frac{i}{\hbar}\int_b^x dx\, p(x) - i\frac{\pi}{4}}$$

$\Rightarrow$ F.C. (A) − i(B)

$$\psi^{II} = C\left(\frac{1}{2|p|^{1/2}} e^{-|\tilde{w}|} - \frac{i}{|p|^{1/2}} e^{|\tilde{w}|}\right)$$

$$\simeq -i\frac{C}{|p|^{1/2}} e^{|\tilde{w}|} = -i\frac{C}{|p|^{1/2}} e^{\frac{1}{\hbar}\int_x^b dx\,|p(x)|}$$

$$= -i\frac{C}{|p|^{1/2}}\, e^{\frac{1}{\hbar}\int_a^b dx\,|p|}\; e^{-\frac{1}{\hbar}\int_a^x dx\,|p|}$$

$\Rightarrow$ F.C. (A)

$$\psi^{(I)} = -\frac{iC}{\sqrt{p}}\, 2\cos\left(|w(a,x)| - \frac{\pi}{4}\right) \cdot e^{\frac{1}{\hbar}\int_a^b dx\,|p|}$$

$$= \left(-iC\, e^{\frac{1}{\hbar}\int_a^b dx\,|p|}\right)\left(\frac{1}{\sqrt{p}} e^{\frac{i}{\hbar}\int_a^x dx\, p + \frac{\pi}{4}i} + \frac{1}{\sqrt{p}} e^{-\frac{i}{\hbar}\int_a^x dx\, p + i\frac{\pi}{4}}\right)$$

Onda inc. — onda riflessa

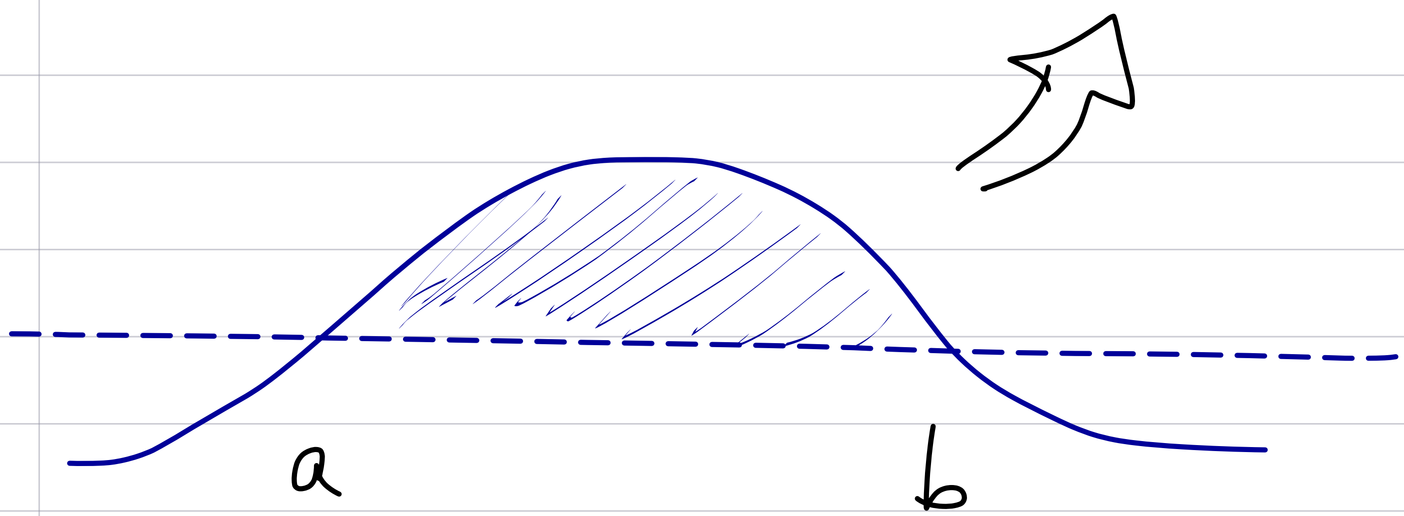
Dividendo tutto con $C \cdot e^{\frac{1}{\hbar}\int_a^b dx\,|p|}$ si ha:

$$\psi(x) \xrightarrow[x\to-\infty]{} \frac{1}{\sqrt{p}} e^{\frac{i}{\hbar}\int_a^x dx\, p + \frac{\pi}{4}i} + \frac{1}{\sqrt{p}} e^{-\frac{i}{\hbar}\int_a^x dx\, p + \frac{\pi}{4}i}$$

$$\xrightarrow[x\to+\infty]{} i\left(e^{-\frac{1}{\hbar}\int_a^b dx\,|p|}\right) \cdot \frac{1}{\sqrt{p}} e^{\frac{i}{\hbar}\int_b^x dx\, p - \frac{\pi}{4}i}$$

onda trasmessa

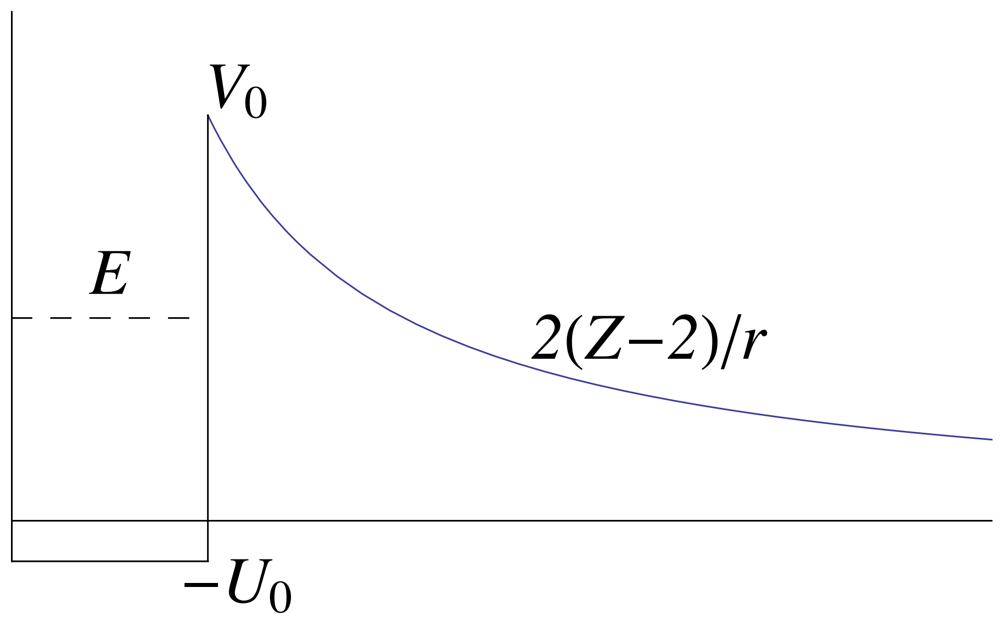
$$\therefore \; P^{trasm} = J_I / J_{I'} = e^{-\frac{2}{\hbar}\int_a^b dx\, |p|}$$

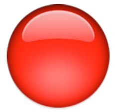


$$\text{Effetto tunnel} \sim e^{-\frac{2}{\hbar}\underbrace{\int_a^b dx\, |p|}_{\text{azione ridotta}}}$$

↑ azione ridotta

Esempio: decadimento α (modello semplice)

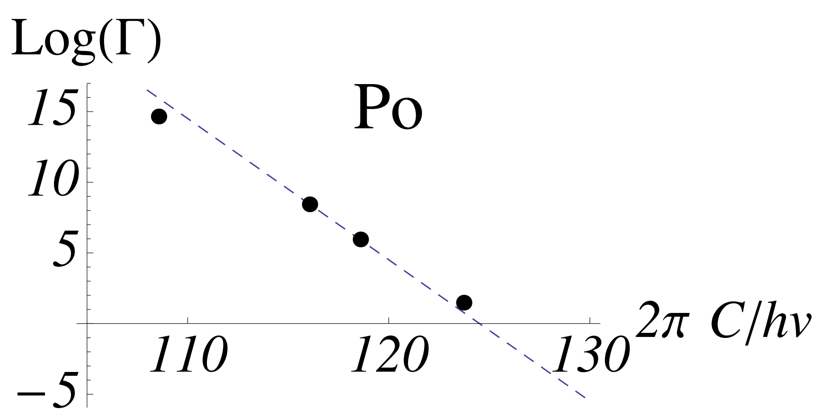


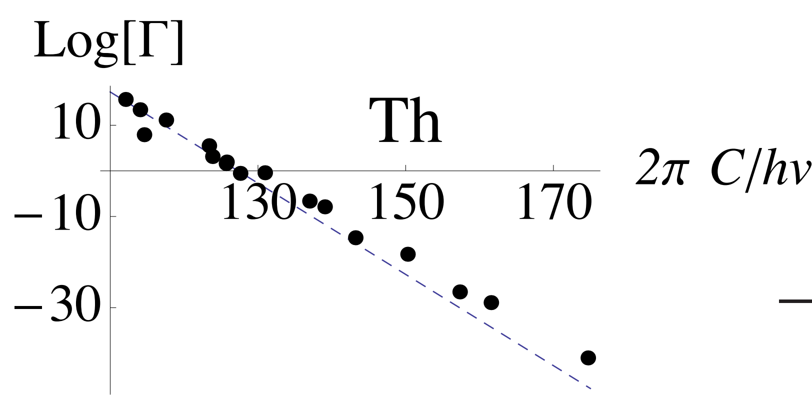


$$\gamma = \mathcal{N} \times P \ , \quad \dashrightarrow \quad \Gamma = \hbar\,\gamma = \frac{\hbar}{T}\,P \ .$$

$$\psi = \frac{1}{\sqrt{4\pi}}\,\frac{A}{r}\,\sin(kr) = \frac{1}{\sqrt{4\pi}}\,\frac{A}{2i\,r}\left[e^{ikr} - e^{-ikr}\right] . \quad \dashrightarrow \quad v/2r_0 = 1/T$$

$$P = \exp\left[-2\sigma(r_0, r_1)\right] = \exp\left[-\frac{2}{\hbar}\int_{r_0}^{r_1} \sqrt{2m\,(\frac{2(Z-2)e^2}{r} - E)}\,dr\right] .$$





Z(A)	$T_{1/2}$	E(MeV)	Z(A)	$T_{1/2}$	E(MeV)
Po(212)	3.0×10^{-7} s	8.95	Th(219)	0.11×10^{-6} s	9.34
Po(214)	1.5×10^{-4} s	7.83	Th(220)	$10. \times 10^{-6}$ s	8.79
Po(215)	1.8×10^{-3} s	7.50	Th(221)	$2.8\,10^{-3}$ s	7.98
Po(216)	0.158 s	6.89	Th(224)	1.05 s	7.085
Th(212)	0.03 s	7.92	Th(225)	8.72 m	6.47
Th(213)	0.14	7.69	Th(226)	30.6 m	6.28
Th(214)	0.10 s	7.68	Th(227)	18.72 d	5.92
Th(215)	1.2 s	7.46	Th(228)	1.91 y	5.38
Th(217)	0.25×10^{-3} s	9.25	Th(229)	7340 y	4.91
Th(218)	0.11×10^{-6} s	9.67	Th(230)	77×10^{3} y	4.65
			Th(232)	14.1×10^{9} y	3.98

THE END