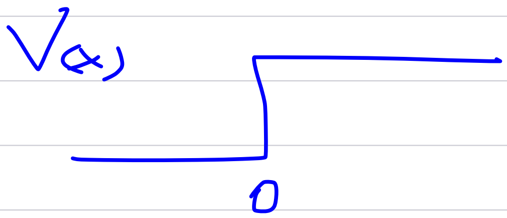
Eq. di Schrödinger in 1D.

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

- $\|\psi\| < \infty \rightarrow |\psi| < x^{-1/2}$ $\quad x\to\infty$ (stati legati)
- Continuità di ψ e ψ' attraverso una discontinuità finita di $V(x)$.

$\because$



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

$$\int_{-\epsilon}^{\epsilon} \cdot \Rightarrow -\frac{\hbar^2}{2m}(\psi'_+ - \psi'_-) + \cancel{V_0\,\epsilon\,\psi_0} = \cancel{E\psi_0\,\epsilon}$$

$$\therefore\ \psi'_+ = \psi'_-.$$

Teo $\quad E_n \geq V_{min}$. ... NO

$$H\psi_n = \left(\frac{p^2}{2m} + V\right)\psi = E\psi$$

$$\langle E\rangle_\psi = \frac{1}{2m}\underbrace{\langle p^2\rangle_\psi}_{\geq 0} + \langle V\rangle_\psi \geq V_{min} \quad \text{ok}$$

$$\langle A^\dagger A\rangle \geq 0$$

Teo. Nondegenerazione di stati legati 1D.

Supp. per assurdo, che ci siano due stati ψ_1 e ψ_2, con la stessa energia E.

$$-\frac{\hbar^2}{2m}\psi_1'' + V\psi_1 = E\psi_1$$
$$\psi_2 \qquad\qquad \psi_2 \qquad\qquad \psi_2$$

$$\Rightarrow \quad \psi_2\psi_1'' - \psi_1\psi_2'' = 0$$

$$\Rightarrow \quad \psi_2\psi_1' - \psi_1\psi_2' = \text{cost.}$$

$\text{cost} = 0$, perché $\psi \xrightarrow[|x|\to\infty]{} 0$

$$\therefore \quad \frac{\psi_1'}{\psi_1} = \frac{\psi_2'}{\psi_2} \Rightarrow \psi_1 = \text{cost.}\,\psi_2 .$$

Andamento generale della funz. d'onda.

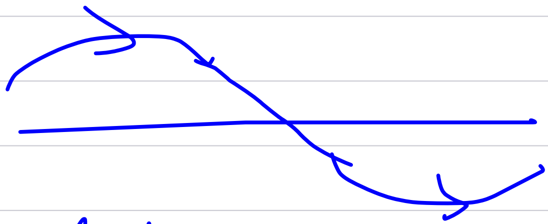
$$-\frac{\hbar^2}{2m}\psi'' = (E - V(x))\psi.$$

$E > V(x)$ (regione classica)

$$\psi'' = -\frac{2m}{\hbar^2}\underbrace{(E-V(x))}_{>0}\psi$$

$< 0 \quad \psi > 0$

$> 0 \quad \psi > 0$

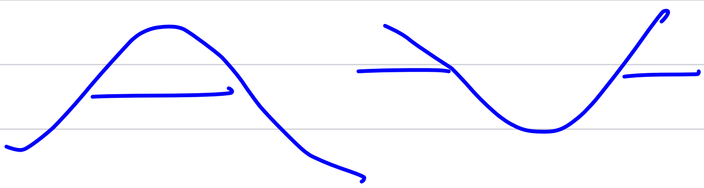


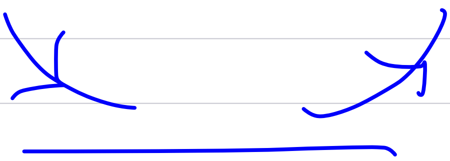
andam. oscillatorio

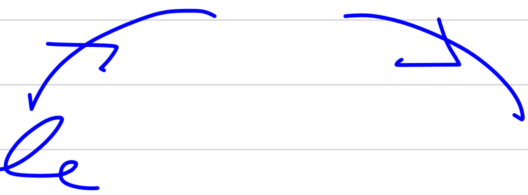
$E < V(x)$ (classicam. inaccessibile)

$\psi'' > 0 \quad \psi > 0$

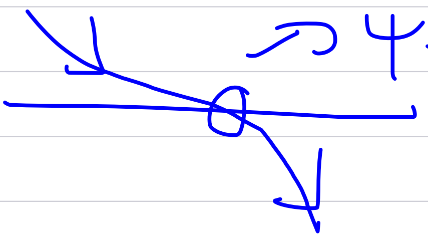
$\psi'' < 0 \quad \psi < 0$



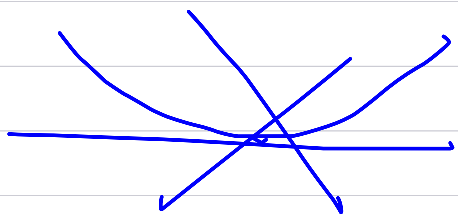




andamento instabile.



$\Rightarrow \psi'' = 0$



Teorema di oscillazione.

In 1D l'n-simo stato legato $\psi_n(x)$ $n = 1, 2, 3 \ldots$

ψ_n dell-

ha $(n-1)$ nodi.

Stati legati 1D.

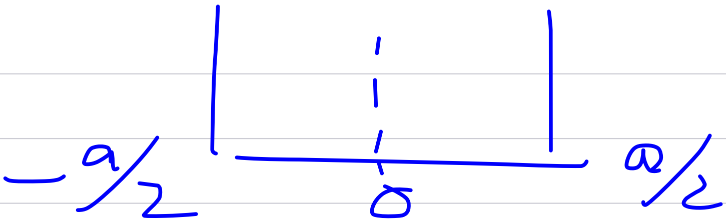
Particella confinata a $[0, a]$

$$V(x) = \infty \qquad x<0\,;\; x>a$$
$$ = 0 \qquad 0<x<a.$$

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

ψ

Rianalisi con



$V(-x)=V(x)$

$V(-x)=V(x) \Rightarrow H(x,p)$ $\boxed{\text{: inv. per parità}}$

$\Pi H \Pi = H(-x,-p)$; $\Pi \psi(x) = \psi(-x)$

Π = operatore di parità. $\Pi^2 = \mathbb{1}$

Ora $H\psi_n = E_n \psi_n$

$\Rightarrow \Pi H \Pi^{-1} \Pi \psi_n = E_n \Pi \psi_n$

$\therefore H(x,p)\,\psi_n(-x) = E_n \psi_n(-x)$

$\therefore$ $\psi_n(x)$ e $\psi_n(-x)$ appartengono allo stesso autoval. E_n

Teo. Nondeg $\Rightarrow \psi_n(-x) = c\,\psi_n(x)$

$c^2 = 1 \Rightarrow c = \pm 1$!

Sol. pari o dispari. Simmetria

(i) Soluz pari.

$\psi'' = -k^2 \psi$, $k = \frac{\sqrt{2mE}}{\hbar}$

$\psi = A \cos kx$

$0 = \psi\left(\frac{a}{2}\right) = A \cos\frac{ka}{2}$ $\therefore$ $\frac{ka}{2} = \frac{2n+1}{2}\pi$

$k = \frac{(2n+1)\pi}{a}$ $(n = 0, 1, 2 \dots)$ (*)

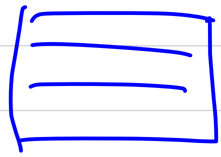
(ii) Sol. dispari:

$$\psi = A \sin kx$$

$$\psi\left(\frac{a}{2}\right) = A \sin\frac{ka}{2} = 0 \quad \therefore \quad \frac{ka}{2} = \pi n, \quad n = 1, 2, \dots$$

$$k = \frac{2\pi n}{a} \qquad (n = 1, 2 \dots) \qquad \cancel{(**)}$$

$$(*), (**) \Rightarrow \quad k = \frac{\pi n}{a} \qquad (n = 1, 2, 3 \dots) \quad \text{ok.}$$



Applicazione: Gas 1D

$$E_{n_1 \dots n_N} = \frac{\pi^2 \hbar^2}{2ma^2}\left(n_1^2 + n_2^2 + \dots n_N^2\right)$$

$$P_{n_1, n_2 \dots} = N e^{-E/kT}$$

$$\langle E_{n_1 \dots} \rangle = N \sum_n \frac{\pi^2 \hbar^2}{2ma^2} n^2 e^{-\frac{\pi^2\hbar^2 n^2}{2ma^2}/kT} \Big/ \sum_n e^{-\frac{\pi^2 \hbar^2 n^2}{2ma^2}/kT}$$

$$kT \gg \frac{\hbar^2}{ma^2} \qquad E_n = \frac{\pi^2\hbar^2}{2ma^2} n^2, \qquad \sqrt{\frac{\pi^2\hbar^2}{2ma^2}}\, n \equiv x$$

$$\langle E_N \rangle \simeq N \int_0^\infty dx\, x^2 e^{-x^2/kT} \Big/ \int dx\, e^{-x^2/kT} = \frac{NkT}{2}$$

$$\therefore \quad C = \partial \langle E \rangle / \partial T \simeq Nk/2$$

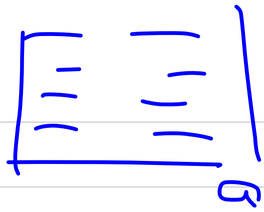
$$T \to 0 \quad \langle E \rangle \simeq \frac{\pi^2 \hbar^2}{2ma^2} N^2 \quad \therefore \quad C = \frac{\partial \langle E \rangle}{\partial T} = 0.$$

$$\langle E \rangle = N\alpha\left(e^{-\alpha/kT} + 4e^{-4\alpha/kT} + \dots\right) \Big/ \left(e^{-\alpha/kT} + e^{-4\alpha/kT} + \dots\right)$$

$$\simeq N\alpha\left(1 + 3 e^{-3\alpha/kT} + \dots\right)$$

$$\frac{\partial E}{\partial T} \simeq 3N\alpha \cdot \frac{3\alpha}{kT^2} e^{-3\alpha/kT} \longrightarrow$$

$$\frac{\partial \langle E_{n_1 \dots} \rangle}{\partial a} = -\frac{2}{a}\langle E_{n_1 \dots} \rangle$$



$$\langle E_{n..} \rangle \Big|_{a+\delta a} = \langle E_{n..} \rangle + \frac{\partial E}{\partial a}\,\delta a$$

" pressione

$$\therefore\ P = -\left\langle \frac{\partial E_{n_1 \dots}}{\partial a} \right\rangle = +\frac{2}{a}\langle E_{n_1 \dots} \rangle$$

$$= +\frac{2}{a}\frac{NkT}{2} = +\frac{1}{a}NkT$$

$$\boxed{PV = NkT}$$ ✓.

Eq. di gas ideale.

Buco finito.

Inf. $\psi'' = -k^2\psi \Rightarrow \sin kx,\ \cos kx$

Est. $\psi'' = \kappa^2\psi,\quad \kappa^2 = \frac{2m(V_0-E)}{\hbar^2}$

$\psi = e^{\pm\kappa x} \rightarrow \psi = e^{-\kappa x} \quad x > a/2$

$= e^{\kappa x} \quad x < -a/2.$

Sol. pari

$\psi^{i} = A\cos kx \qquad \psi^{est} = B e^{-\kappa x} \quad x > a/2$

$= B e^{\kappa x} \quad x < -\frac{a}{2}$

Cond. raccordo

$x = a/2$, ψ: $A\cos\frac{ka}{2} = B e^{-\kappa a/2}$ (1)

ψ': $-Ak\sin\frac{ka}{2} = -B\kappa e^{-\kappa a/2}$ (2)

(1)/(2) $\Rightarrow$ $-k\tan\frac{ka}{2} = -\kappa \qquad \xi^2 + \eta^2 = \frac{a^2}{4}(k^2 + \kappa^2)$

$\frac{ka}{2} = \xi\ ;\ \frac{\kappa a}{2} = \eta \Longrightarrow = \frac{mV_0 a^2}{2\hbar^2}$

$$\begin{cases} \eta = \xi\tan\xi \\ \xi^2 + \eta^2 = \frac{mV_0 a^2}{2\hbar^2} \end{cases}$$

Sol. dispari

$\psi^{int} = A \sin kx \; ; \quad \psi^{est} = B e^{-\kappa x} \quad x > a/2$

$= -B e^{\kappa x} \quad x < -a/2.$

Cond. raccordo $x = a/2$

$$A \sin \frac{ka}{2} = B e^{-\kappa a/2}$$

$$k A \cos \frac{ka}{2} = -\kappa B e^{-\kappa a/2}$$

$\Rightarrow \quad k \cot \frac{ka}{2} = -\kappa. \qquad ka = \xi$

$\kappa a = \eta.$

$$\begin{cases} \eta = -\xi \cot \xi . \\ \xi^2 + \eta^2 = \dfrac{m V_0 a^2}{2\hbar^2} . \end{cases}$$