

Teo. de Ehrenfest

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H} \psi \quad (1)$$

$$\text{con } \hat{H} = \frac{\hat{p}^2}{2m} + V \quad (2)$$

sea $\hat{A}$ operador arbitrario

$$\frac{d}{dt} \langle A \rangle = \frac{d}{dt} \int \psi^* A \psi = \int \frac{\partial \psi^*}{\partial t} A \psi + \int \psi^* \frac{\partial A}{\partial t} \psi + \int \psi^* A \frac{\partial \psi}{\partial t}$$

$$(1) \rightarrow \frac{\partial \psi}{\partial t} = -\frac{i}{\hbar} \hat{H} \psi, \quad \text{y} \quad \frac{\partial \psi^*}{\partial t} = \frac{i}{\hbar} \hat{H} \psi^* \quad (3)$$

$$\begin{aligned} \Rightarrow \frac{d}{dt} \langle A \rangle &= \frac{i}{\hbar} \langle \hat{H} \psi | A \psi \rangle + \langle \psi | \frac{\partial A}{\partial t} \psi \rangle - \frac{i}{\hbar} \langle \psi | A \hat{H} \psi \rangle \\ &= \frac{i}{\hbar} \langle \psi | [\hat{H}, \hat{A}] \psi \rangle + \langle \frac{\partial A}{\partial t} \rangle \end{aligned} \quad (4)$$

$$\frac{d \langle \hat{A} \rangle}{dt} = \frac{i}{\hbar} \langle [\hat{H}, \hat{A}] \rangle + \langle \frac{\partial A}{\partial t} \rangle \quad (5)$$

$$([A, B] = AB - BA)$$

Aplicaciones: $\hat{A} = \hat{x}$

$$[\hat{H}, \hat{x}] = \left[\frac{\hat{p}^2}{2m} + V, \hat{x} \right] = \frac{1}{2m} [\hat{p}^2, \hat{x}] = \frac{1}{2m} (\hat{p}^2 \hat{x} - \hat{x} \hat{p}^2)$$

$$(\hat{p}^2 \hat{x} - \hat{x} \hat{p}^2) \psi = -\hbar^2 \frac{d^2}{dx^2} (x \psi) + \hbar^2 x \frac{d^2}{dx^2} \psi$$

$$= -\hbar^2 (2\psi' + x\psi'' - x\psi'') = -2\hbar^2 \frac{\partial \psi}{\partial x}$$

$$\therefore [H, x] = \frac{1}{2m} \cdot (-2)\hbar^2 \frac{\partial \psi}{\partial x} = -\frac{\hbar^2}{m} \frac{\partial \psi}{\partial x}$$

$$\Rightarrow \frac{d\langle x \rangle}{dt} = \left\langle \frac{i}{\hbar} \left(-\frac{\hbar^2}{m} \right) \frac{\partial \psi}{\partial x} \right\rangle = \frac{\langle p \rangle}{m}$$

$$\boxed{\frac{d\langle x \rangle}{dt} = \frac{\langle p \rangle}{m}} \quad (6)$$

$$(2) \quad \check{A} = \check{P}$$

$$[H, p] = \left[\frac{p^2}{2m} + V, p \right] = [V(x), p]$$

$$\begin{aligned} [V, p] \psi &= (Vp)\psi - (pV)\psi = V(-i\hbar \frac{\partial}{\partial x})\psi + i\hbar \frac{\partial}{\partial x} (V\psi) \\ &= -i\hbar \underbrace{(\frac{\partial \psi}{\partial x}) V} + i\hbar \underbrace{(\frac{\partial V}{\partial x}) \psi} + i\hbar V \underbrace{(\frac{\partial \psi}{\partial x})} \end{aligned}$$

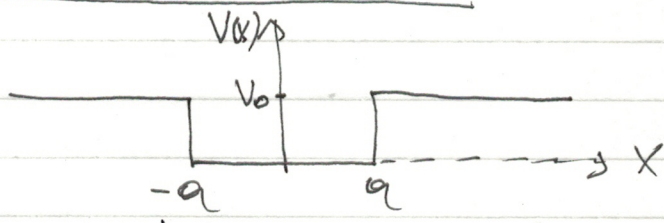
$$\Rightarrow [V, p] = i\hbar \frac{\partial V}{\partial x}$$

$$\Rightarrow \boxed{\frac{d\langle p \rangle}{dt} = \frac{i}{\hbar} \cdot i\hbar \frac{\partial V}{\partial x} = -\frac{\partial V}{\partial x} = F} \quad (7)$$

$$(6), (7) \Rightarrow \boxed{F = m \frac{d^2 \langle x \rangle}{dt^2}} \quad (8)$$

EL pozo cuadrado unidimensional

$$V(x) = \begin{cases} V_0 & |x| > a \\ 0 & |x| < a \end{cases}$$



Consideremos el caso $E < V_0$: $u'' = -\frac{2m}{\hbar^2}(E - V)u$ (4)

$|x| > a$: $u'' = \frac{2m}{\hbar^2}(V_0 - E)u \equiv \alpha^2 u \Rightarrow u \propto e^{\pm \alpha x}$

$|x| < a$: $u'' = -\frac{2mE}{\hbar^2}u \equiv -k^2 u \Rightarrow u \propto \{ \cos kx, \sin kx \}$

manda que $\psi \rightarrow 0$ cuando $|x| \rightarrow \infty$

$\Rightarrow u(x) = Ae^{\alpha x} \quad x < -a$

$u(x) = Be^{-\alpha x} \quad x > a$

$u(x) = C \cos(kx) + D \sin(kx) \quad |x| < a$

(5)

Cont. de u en $x = \pm e$:

$$x = -e \quad A e^{-\alpha e} = C \cos(ke) - D \sin(ke) \quad (6)$$

$$x = +e \quad B e^{-\alpha e} = C \cos(ke) + D \sin(ke) \quad (7)$$

$$\text{sumando: } (A+B) e^{-\alpha e} = 2C \cos(ke) \quad (6')$$

$$\text{restando: } (B-A) e^{-\alpha e} = 2D \sin(ke) \quad (7')$$

Continuidad de u' en $x = \pm e$:

$$x = -e \quad \alpha A e^{-\alpha e} = Ck \sin(ke) + Dk \cos(ke) \quad (8)$$

$$x = +e \quad -\alpha B e^{-\alpha e} = -Ck \sin(ke) + Dk \cos(ke) \quad (9)$$

$$\text{sumando: } \alpha (A-B) e^{-\alpha e} = 2Dk \cos(ke) \quad (8')$$

$$\text{restando: } \alpha (A+B) e^{-\alpha e} = 2Ck \sin(ke) \quad (9')$$

$$\frac{(8')}{(7')} \quad -\alpha = k \cot(ke) \quad [\text{si } A \neq B \text{ y } D \neq 0] \quad (10)$$

$$\frac{(9')}{(6')} \quad \alpha = k \tan(ke) \quad [\text{si } A \neq -B \text{ y } C \neq 0] \quad (11)$$

(10) y (11) no pueden ser válidas al mismo tiempo.

Caso I: F.C. (10) no vale porque $A=B$ y $D=0$

$$\Rightarrow \boxed{\alpha = k \tan(ke)}$$

$$u(x) = \begin{cases} A e^{\alpha x} & x < -e \\ C \cos(kx) & -e < x < e \\ A e^{-\alpha x} & x > e \end{cases}$$

el m es por

Caso II: (ii) No es válido porque $A = -B$ y $C = 0$

$$\Rightarrow \boxed{-\alpha = K \cot(ka)}$$

$$u(x) = \begin{cases} A e^{\alpha x} & x < -a \\ D \sin(Kx) & -a < x < a \\ -A e^{-\alpha x} & x > a \end{cases}$$

$u(x)$ es
impar

Recordemos que:

$$K = \sqrt{2mE/\hbar^2} \quad y \quad \alpha = \sqrt{2m(V_0 - E)/\hbar^2}$$

$$\Rightarrow \boxed{K^2 + \alpha^2 = \frac{2mV_0}{\hbar^2} \equiv \beta^2}$$

$$\text{let } \alpha = K \tan(ka)$$

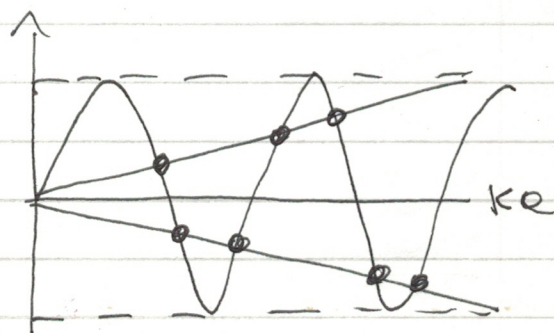
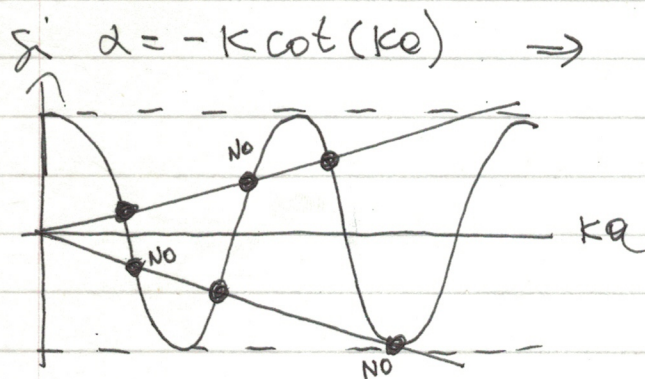
$$\Rightarrow K^2 + K^2 \tan^2(ka) = \beta^2$$

$$\Rightarrow K^2 \sec^2(ka) = \beta^2$$

$$\Rightarrow \begin{cases} \cos(ka) = \pm \frac{K a}{\beta a} \\ \sin(ka) = \pm \frac{K a}{\beta a} \end{cases}$$

soluc.
PAR

soluc.
impar



$$ka \in [0, \frac{\pi}{2}] \cup [\pi, \frac{3\pi}{2}] \cup [2\pi, \frac{5\pi}{2}] \cup \dots$$

$\uparrow$
con $\tan(ka) > 0$

con $\cot(ka) < 0$

$$ka \in [\frac{\pi}{2}, \pi] \cup [\frac{3\pi}{2}, 2\pi] \cup [\frac{5\pi}{2}, 3\pi] \cup \dots$$

Exemplo. $V_0 = 10 \text{ (ev)}$; $a = 10^{-7} \text{ (cm)}$. Calcule as energias de autoenergias de elétrons livres?

$$\beta a = \left[\frac{2m V_0 a^2}{\hbar^2} \right]^{1/2} = 16.2$$

$$m = 9.1 \times 10^{-28} \text{ (g)}$$

$$V_0 = 10 \times 1.602 \times 10^{-12} \text{ (erg)}$$

$$\hbar = 1.054 \times 10^{-27} \text{ (erg.s)}$$

$$\text{Condição } ka, E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2ma^2} (ka)^2 = E_0 (ka)^2$$

$$\text{donde } E_0 = \hbar^2 / 2ma^2 = 0.038102 \text{ [ev]}$$

$$\cos(ka) = \pm \frac{ka}{16.2} \Rightarrow \cos(x) = \pm \frac{x}{16.2}$$

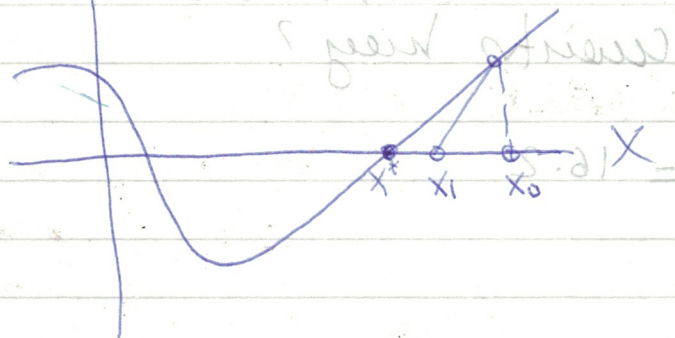
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$\cos(x) = \pm \frac{x}{16.2}$	$\sin(x) = \pm \frac{x}{16.2}$
x	x
1.47935 ✓	2.95797 ✓
1.67434 ✗	3.34988 ✗
4.43508 ✓	5.90977 ✓
5.02797 ✗	6.71026 ✗
7.38092 ✓	8.84706 ✓
8.39903 ✗	10.0978 ✗
10.306 ✓	11.7545 ✓
13.1862 ✓	13.558 ✗
15.3905 ✗	14.5872 ✓
15.9008 ✓	

Energias	$\frac{\hbar^2 k^2}{2ma^2} n^2$
0.0834 (ev)	0.094
0.333 (ev)	0.376
0.7495 (ev)	0.846
1.3307 (ev)	1.504
2.0757 (ev)	2.350
2.9823 (ev)	3.384
4.047 (ev)	4.607
5.2649 (ev)	6.02
6.6250 (ev)	7.615
8.1076 (ev)	9.401
9.6332 (ev)	11.376

Newton-Raphson



$$0 = f(x) = f(x_0 + \Delta x) \approx f(x_0) + \Delta x f'(x_0)$$

$$\Delta x = -\frac{f(x_0)}{f'(x_0)}$$

$$x \approx x_0 - \frac{f(x_0)}{f'(x_0)} \quad \text{and here}$$

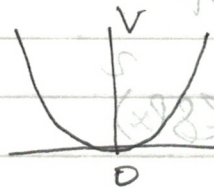
$$x_{\text{new}} = x_{\text{old}} - \frac{f(x_{\text{old}})}{f'(x_{\text{old}})}$$

$f(x)$	$f'(x)$	$x_{\text{new}} = x_{\text{old}} - \frac{f(x_{\text{old}})}{f'(x_{\text{old}})}$	x	x
11.349	0.0335	8.1049	12.3802	12.3802
0.4101	0.01049	8.1049	13.228	13.228
2.012	0.02520	8.1049	10.309	10.309
6.05	0.02564	8.1049	8.34903	8.34903
4.04	0.0104	8.1049	5.05	5.05
3.384	0.00553	8.1049	2.0085	2.0085
0.320	0.00270	8.1049	0.00270	0.00270
1.201	0.00270	8.1049	0.00270	0.00270
0.4101	0.00270	8.1049	0.00270	0.00270
0.0335	0.00270	8.1049	0.00270	0.00270

>> Newton-Raphson

$$\underline{E(\text{oscilador armónico})} + \langle \hat{x} \rangle \frac{f}{m} = E$$

$$V(x) = \frac{1}{2} k x^2$$

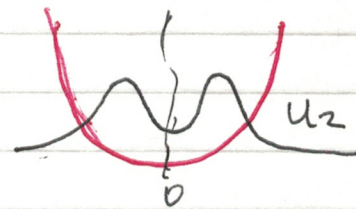
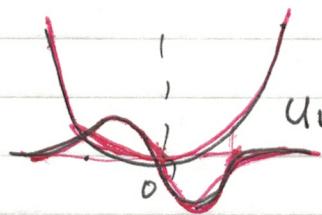
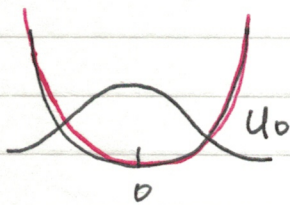


$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} k x^2 \right) u = E u \quad (1)$$

$$\left(\frac{d^2}{dx^2} - \frac{m k x^2}{\hbar^2} \right) u = -\frac{2mE}{\hbar^2} u \quad (2)$$

$$b \quad \left(\frac{d^2}{dx^2} - a^2 x^2 \right) u = -b u \quad (3)$$

Situación es parecida a un pozo cuadrado profundo. Además $V(x)$ es par $\Rightarrow$ definito.
poseen paridad definida.



$$E = \frac{\langle \hat{p}_x^2 \rangle}{2m} + \frac{1}{2} k \langle x^2 \rangle$$

$$\text{Si } E=0 \Rightarrow \langle x^2 \rangle=0 \text{ y } \langle \hat{p}_x^2 \rangle=0$$

$$\Rightarrow \Delta x = 0 \wedge \Delta p_x = 0 \rightarrow \leftarrow$$

$$(\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sqrt{\langle x^2 \rangle} \wedge \Delta p_x = \sqrt{\langle p_x^2 \rangle - \langle p_x \rangle^2} = \sqrt{\langle p_x^2 \rangle})$$

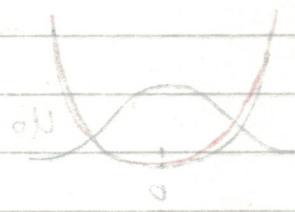
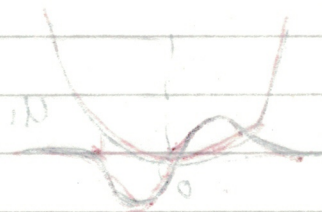
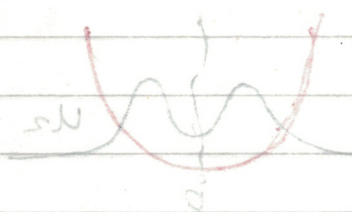
$$E = \frac{m\omega^2}{2} \langle x^2 \rangle + \frac{\langle p_x^2 \rangle}{2m}$$

$$= \frac{m\omega^2}{2} (\Delta x)^2 + \frac{1}{2m} (\Delta p_x)^2$$

umso $\Delta x \Delta p_x \geq \hbar/2$

$$E \geq \frac{m\omega^2}{2} (\Delta x)^2 + \frac{\hbar^2}{8m (\Delta x)^2}$$

$$\boxed{E_{\min} = \frac{\hbar\omega}{2}}$$



$$E = \frac{\hbar\omega}{2} + \frac{1}{2} \hbar\omega$$

$$E = 0 \Rightarrow \langle x^2 \rangle = 0 \Rightarrow \langle p_x^2 \rangle = 0$$



$$\Rightarrow \Delta x = 0 \vee \Delta p_x = 0 \Rightarrow \Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sqrt{\langle x^2 \rangle} = \Delta p_x = \sqrt{\langle p_x^2 \rangle - \langle p_x \rangle^2} = \sqrt{\langle p_x^2 \rangle}$$

$$\left(\frac{d^2}{dx^2} - a^2 x^2\right) u = -bu \quad (1)$$

reescribi como:

$$\left[\left(\frac{d}{dx} - ex\right)\left(\frac{d}{dx} + ex\right) - a\right] u = -bu \quad (2)$$

Dem. $\left(\frac{d}{dx} - ex\right)(u' + exu) - eu$

$$u'' + \cancel{ax} + \cancel{ax}u' - \cancel{ax}u' - a^2 x^2 u - eu$$

$$u'' - a^2 x^2 u \quad \checkmark \quad //$$

o sea, $\left(\frac{d}{dx} - ex\right)\left(\frac{d}{dx} + ex\right)u = (-b+a)u \quad (3)$

Aplicar $\left(\frac{d}{dx} + ex\right)$ a ambos lados de (3):

$$\left(\frac{d}{dx} + ex\right)\left(\frac{d}{dx} - ex\right)\underbrace{\left(\frac{d}{dx} + ex\right)u}_{u'} = -(b-a)\underbrace{\left(\frac{d}{dx} + ex\right)u}_{u'} \quad (4)$$

$$\left(\frac{d}{dx} + ex\right)\left(\frac{d}{dx} - ax\right)u' = -(b-a)u' \quad (4')$$

desarrollando $\nearrow$

$$\left(\frac{d}{dx} + ex\right)\left(\frac{du'}{dx} - axu'\right) = \frac{d^2 u'}{dx^2} - au' - ex \cancel{\frac{du'}{dx}} + ax \cancel{\frac{du'}{dx}} - a^2 x^2 u'$$

$$= \frac{\hbar^2}{2m} \frac{d^2 u'}{dx^2} - \frac{1}{2} \alpha^2 x^2 u' - \epsilon u'$$

$$\therefore \frac{\hbar^2}{2m} \frac{d^2 u'}{dx^2} - \frac{1}{2} \alpha^2 x^2 u' = - (b - 2a) u' \quad (5)$$

mismo ec. que (1) con distinto b , y u' .

Luego si def: $b - 2a = (2m/\hbar^2) E' \rightarrow E'$ es la energía de un Osc. Arm. cuyo fn. de onda es u' .

$$\frac{2mE}{\hbar^2} - \frac{2m\omega}{\hbar} = \frac{2mE'}{\hbar^2}$$

$$\Rightarrow \boxed{E' = E - \hbar\omega} \quad (6)$$

"operador de bajada"

$\therefore$ Si $u(x)$ es autofn. del op. de energía del Osc. Arm.
 $u'(x) \equiv (d/dx + \alpha x) u(x)$ es también autofn. del mismo operador, con autovalor menor q' el autov. de $u(x)$ es una cantidad $\hbar\omega$. $\Rightarrow$ se puede generar toda una serie de autofns. equiespaciados en $\hbar\omega$.

Como todas las energías permitidas son positivas $\rightarrow$ debe haber una energía mínima > 0 , E_0 con autofn. u_0

$$y \quad \left(\frac{d}{dx} + \alpha x \right) u_0 = 0$$

$$\Rightarrow \frac{du_0}{dx} = -\alpha x u_0 \Rightarrow \frac{du_0}{u_0} = -\alpha x dx$$

$$\int \frac{du_0}{u_0} = \int (-\alpha x) dx \Rightarrow \boxed{u_0 = A e^{-\frac{\alpha x^2}{2}}} \quad (7)$$

donde A se det. por normalización.

Reemplazando (7) en (1), hallamos E_0 .

$$\frac{d\psi_0}{dx} = -ax A e^{-\frac{ax^2}{2}}$$

$$\Rightarrow \frac{d^2\psi_0}{dx^2} = -a A e^{-\frac{ax^2}{2}} + a^2 x^2 A e^{-\frac{ax^2}{2}}$$

$$\Rightarrow -a A e^{-\frac{ax^2}{2}} + \cancel{a^2 x^2 A e^{-\frac{ax^2}{2}}} - \cancel{a^2 x^2 A e^{-\frac{ax^2}{2}}} = -b A e^{-\frac{ax^2}{2}}$$

$$\Rightarrow a = b \Rightarrow \frac{m\omega}{\hbar} = \frac{2mE_0}{\hbar^2} \Rightarrow \boxed{E_0 = \frac{1}{2}\hbar\omega} \quad (8)$$

Teniendo la energía más baja E_0 , y su autofn. ψ_0 , hallamos los otros autofn. usando un proc. similar que nos permite generar los autofn. de energías superiores.

Aplicamos el operador $(\frac{d}{dx} - ax)$ a ambas lados de $(\psi')'$.

$$\left(\frac{d}{dx} - ax\right) \underbrace{\left(\frac{d}{dx} + ax\right) \left(\frac{d}{dx} + ax\right) \psi'}_{\psi''} = (-b+a) \underbrace{\left(\frac{d}{dx} - ax\right) \psi'}_{\psi''}$$

$$\text{o sea, } \left(\frac{d}{dx} - ax\right) \left(\frac{d}{dx} + ax\right) \psi'' = (-b+a) \psi''$$

$$\frac{d^2}{dx^2} u'' + a u'' + \cancel{a x \frac{d}{dx} u''} - \cancel{a x \frac{d}{dx} u''} - a^2 x^2 u'' = (-b + a) u''$$

$$\Rightarrow \frac{d^2 u''}{dx^2} - a^2 x^2 u'' = -b u'' \quad (9)$$

$\therefore u''$ es autofn. de la ee. original con autov. $-b$ y por tanto su energía es $\hbar\omega$ mayor que la de u' .

$\Rightarrow$ dada una autofn. y su autovalor, podemos generar la autofn. con el sig. autovalor superior aplicando el operador $(\frac{d}{dx} - ax)$ "operador de subida"

las autoenergías del oscilador cuántico son

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

$$\psi_n(t) = \left(\frac{d}{dx} - ax \right)^n e^{-\frac{ax^2}{2}} e^{-i \frac{E_n t}{\hbar}} \quad (\text{sin normalizar})$$

$$\psi_0 = (a/\pi)^{1/4} e^{-\frac{ax^2}{2}} e^{-i\omega t/2}$$

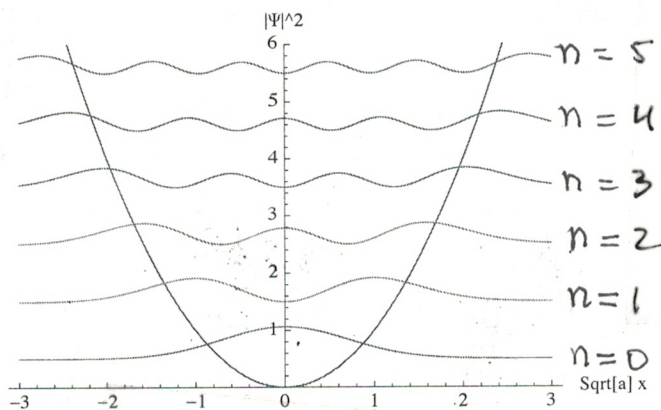
$$\psi_1 = (4a^3/\pi)^{1/4} x e^{-\frac{ax^2}{2}} e^{-3i\omega t/2}$$

$$\psi_2 = (a/4\pi)^{1/4} (2ax^2 - 1) e^{-\frac{ax^2}{2}} e^{-5i\omega t/2}$$

normalizados

(9)

$$\begin{array}{r} 11 \text{ } ^5 \\ \times 5 \\ \hline 55 \\ 55 \\ \hline 550 \end{array}$$



$\therefore \text{Value of } u = 2$

am abab $\Leftarrow$
 0. al renergo
 9 abnaild

not abundant water to the riparian area

$$\omega\left(\frac{1}{n} + \alpha\right) = \alpha \tau$$

$$\frac{S|twi - S_{\theta} - 9}{9} = \frac{S_{\theta} - 9}{9} \quad (\pi|e) = \psi$$

9. $\frac{5}{9} \times (11500) = 7222$

$$\frac{5}{9} \frac{1}{5} = \frac{1}{9} \quad \frac{1}{9} (1 - x_{\text{OS}})^{1/4} = \frac{1}{9}$$