

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

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

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

$$\Rightarrow \frac{d}{dt} \langle A \rangle = \frac{i}{\hbar} \langle \hat{H} \psi | A \psi \rangle + \langle \psi | \frac{\partial A}{\partial t} \psi \rangle - \frac{i}{\hbar} \langle \psi | A \hat{H} \psi \rangle$$

$$= \frac{i}{\hbar} \langle \psi | [\hat{H}, \hat{A}] \psi \rangle + \langle \frac{\partial A}{\partial t} \rangle \quad (4)$$

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

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

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

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

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

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

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

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

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

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

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

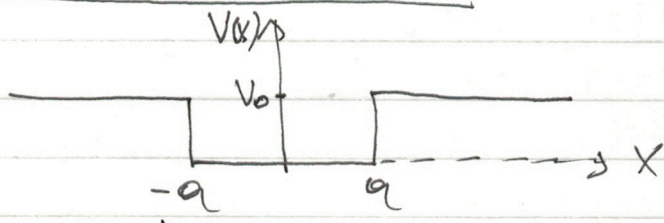
$$\Rightarrow [V, p] = i\hbar \frac{\partial V}{\partial x}$$

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

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

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 válidos 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 $\cos$ es par

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:

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

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

let $\alpha = K \tan(ka)$

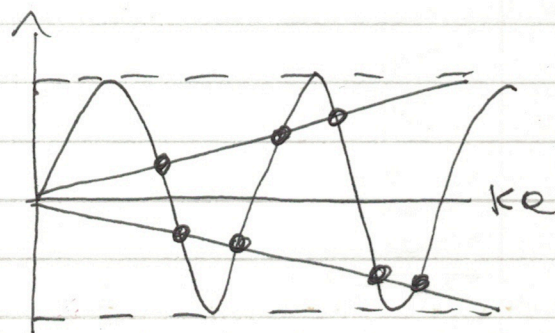
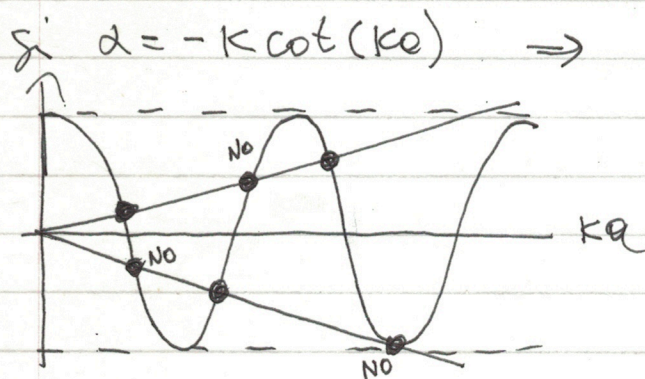
$$\Rightarrow K^2 + K^2 \tan^2(ka) = \beta^2$$

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

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

soluc.
PAR

soluc.
impar



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

con $\tan(ka) > 0$

con $\cot(ka) < 0$

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

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

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

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

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

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

~~Calcule~~ Calcule $k a$, $E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m a^2} (k a)^2 = E_0 (k a)^2$

onde $E_0 = \hbar^2 / 2m a^2 = 0.038102 \text{ [eV]}$

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

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↓

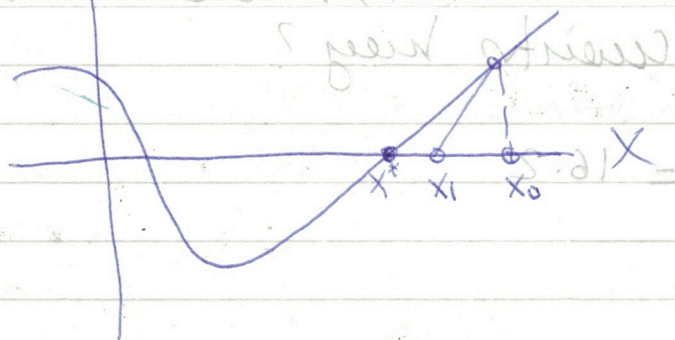
$\cos(x) = \pm \frac{x}{16.2}$ x	$\sin(x) = \pm \frac{x}{16.2}$ x
1.47935 ✓	2.95797 ✓
1.67434 ✗	3.34988 ✗
4.43508 ✓	5.90977 ✓
5.02797 ✗	6.71026 ✗
7.38092 ✓	8.84706 ✓
8.39903 ✗	10.0978 ✗
10.306 ✓	11.7545 ✓
13.1862 ✓	13.558 ✗
15.3905 ✗	14.5872 ✓
15.9008 ✓	

Energias	$\frac{\hbar^2}{8m a^2} n^2$
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

>> Introduza Newton-Raphson.



Newton-Raphson



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

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

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

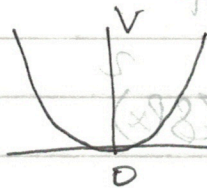
$$x_{\text{new}} = x_{\text{old}} - \frac{f(x_{\text{old}})}{f'(x_{\text{old}})}$$

$f(x)$	$f'(x)$	$x_{\text{new}} = x_{\text{old}} - \frac{f(x_{\text{old}})}{f'(x_{\text{old}})}$	x	x
11.349	0.0335	0.0335	12.000	12.000
0.401	8.1049	0.0498	12.3682	12.3682
0.012	0.0520	0.0520	13.228	13.228
0.005	0.044	0.044	10.306	10.306
0.003	0.0453	0.0453	8.3403	8.3403
0.002	0.0453	0.0453	7.3805	7.3805
0.001	0.0453	0.0453	6.0544	6.0544
0.000	0.0453	0.0453	5.0000	5.0000
0.000	0.0453	0.0453	4.0000	4.0000
0.000	0.0453	0.0453	3.0000	3.0000
0.000	0.0453	0.0453	2.0000	2.0000
0.000	0.0453	0.0453	1.0000	1.0000
0.000	0.0453	0.0453	0.0000	0.0000

>> Introduction to Newton-Raphson

$$\frac{E(\text{oscilador armónico})}{\text{MS}} + \frac{\langle x \rangle \frac{1}{2} \omega m}{\text{MS}} = E$$

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

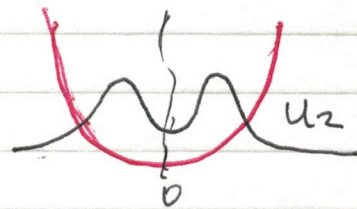
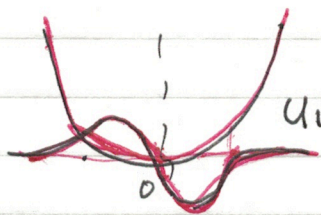
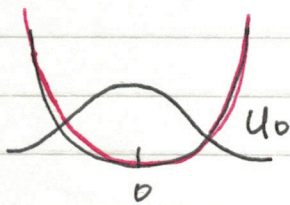


$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} k x^2 \right) u = E u \quad (1)$$

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

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

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



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

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

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

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

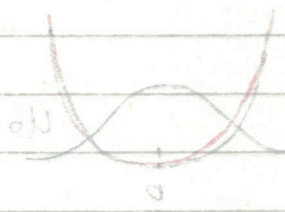
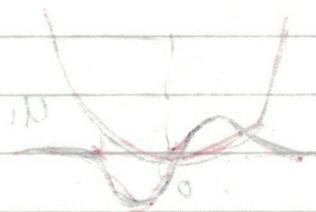
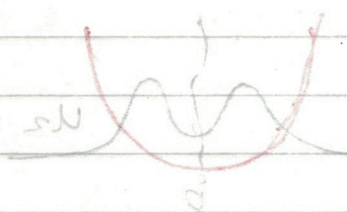
$$E = \frac{m\omega^2}{2} \langle x^2 \rangle + \frac{\langle p_x^2 \rangle}{2m}$$

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

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

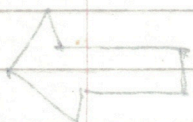
$$\Rightarrow E \geq \frac{m\omega^2}{2} (\Delta x)^2 + \frac{\hbar^2}{8m (\Delta x)^2}$$

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



$$E = \frac{\hbar\omega}{2} + \frac{1}{2} \hbar\omega = \frac{3}{2} \hbar\omega$$

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



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

$$\Delta p_x = \sqrt{\langle p_x^2 \rangle - \langle p_x \rangle^2} = \sqrt{\langle p_x^2 \rangle} = \Delta p_x$$

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

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 $\nearrow$

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

$$= \frac{d^2 u'}{dx^2} - a^2 x^2 u' - a u'$$

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

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.
 $u'(x) \equiv (d/dx + ax)u(x)$ 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

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

$$\Rightarrow \frac{du_0}{dx} = -ax u_0 \Rightarrow \frac{du_0}{u_0} = -ax dx$$

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

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 $(4')'$.

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

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

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

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

$\therefore u''$ 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"

los autovalores 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

