Sch_1_num

NUMERICS

Sabemos que la ecuacion se escribe como

$$\boxed{\frac{d^2}{dx^2}\psi = -\frac{2m}{\hbar^2}[E - V(x)]\psi}$$

10^{27} en cgs (muy grande)

Eso se reescribe como

$$\frac{d^2}{dz^2}\psi = -[e - W]\psi$$

Que es la forma adimensional

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}\left(E - \frac{1}{2}Cx^2\right)$$

$$\frac{d^2\psi}{dz^2} = -(e - z^2)\psi$$

Para el oscilar la ecuacion es

$$E = \frac{p^2}{2m} + \frac{C}{2}x^2 \Rightarrow$$

$$\omega_0 = \sqrt{\frac{C}{m}}$$

$$\boxed{E = \frac{1}{2}\hbar\omega_0\varepsilon}$$

Luego dada la frecuencia caracteristica tomamos una energia caracteristica

Reescribimos ahora

$$\frac{d^2\psi}{dx^2} = \left(-\frac{2m}{\hbar^2}\frac{1}{2}\hbar\omega_0\varepsilon + \frac{2m^2}{\hbar^2}\frac{1}{2}\omega_0^2x^2\right)\psi$$

$$\frac{d^2\psi}{dx^2} = \left(-\frac{m}{\hbar}\omega_0\varepsilon + \frac{m^2}{\hbar^2}\omega_0^2x^2\right)\psi$$

$$\frac{d^2\psi}{dx^2} = -\frac{m}{\hbar}\omega_0\left(\varepsilon - \frac{m}{\hbar}\omega_0x^2\right)\psi$$

$$\frac{d^2\psi}{dx^2(\frac{m}{\hbar}\omega_0)} = -\left(\varepsilon - \frac{m}{\hbar}\omega_0x^2\right)\psi$$

con

$$\boxed{z^2 = \frac{m}{\hbar}\omega_0x^2 \Rightarrow x = \left(\frac{\hbar}{m\omega_0}\right)^{1/2}z}$$

Para el oscilador armonico $V(x) = \frac{1}{2}Cx^2 \rightarrow W(z) = z^2$

con

$$\boxed{\begin{aligned} E &= \frac{1}{2}\hbar\omega_0\, \varepsilon \\ x &= \left(\frac{\hbar}{\mu\omega_0}\right) z \\ \omega_0 &= \left(\frac{C}{\mu}\right)^{1/2} \end{aligned}}$$

Algunas definiciones para el calculo numerico

$$z \rightarrow z_j = j \cdot \Delta z$$

$$\psi(z) \rightarrow \psi(z_j) = \psi_j$$

$$W(z) \rightarrow W(z_j) = W_j$$

Aproximamos la derivada como

La derivada de ψ en el punto $(j+\frac{1}{2})\Delta z$ (en el medio de los puntos de grilla j y $(j+1)$)

$$\frac{\psi_{j+1} - \psi_j}{\Delta z}$$

Para la secunda derivada

$$\boxed{\begin{aligned} \left[\frac{d^2}{dz^2}\psi\right]_{z_j} &= \frac{\frac{\psi_{j+1}-\psi_j}{\Delta z} - \frac{\psi_j - \psi_{j-1}}{\Delta z}}{2\Delta z} \\ &= \frac{\psi_{j+1} - 2\psi_j + \psi_{j-1}}{2(\Delta z)^2} \end{aligned}}$$

Lo cual da para $\frac{d^2}{dz^2}\psi = -[e - W]\psi$

$$\boxed{\frac{\psi_{j+1} - 2\psi_j + \psi_{j-1}}{2(\Delta z)^2} = -[e - W_j]\psi_j} \rightarrow$$

$$\psi_{j+1} = -[e - W_j]\psi_j 2(\Delta z)^2 + 2\psi_j - \psi_{j-1}$$

$$\boxed{\psi_{j+1} = (2 - 2(\Delta z)^2[e - W_j])\psi_j - \psi_{j-1}}$$

Suponemos un potencial simétrico → $V(x) = V(-x)$

Para resolver : $\psi_{j+1} = (2 - 2(\Delta z)^2[e - W_j])\psi_j - \psi_{j-1}$

Necesitamos dar valores

Para ψ:

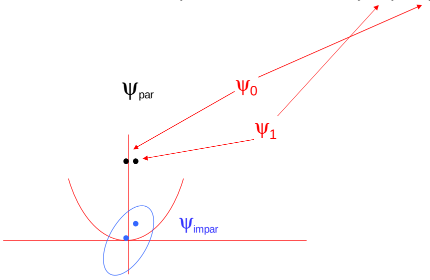
Dado un potencial simétrico luego dado que el observable fundamental es la Probabilidad asociada a $\psi^2(x)$, pero por simetria

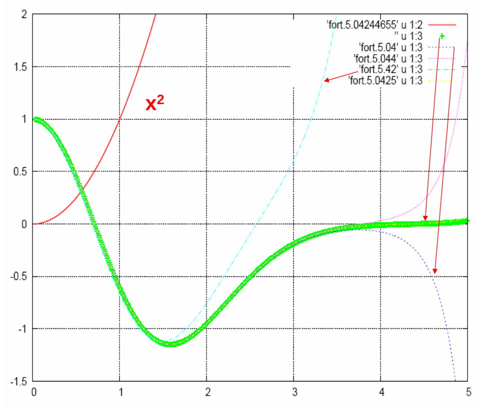
$$\boxed{\begin{aligned} &\Psi^2(x) = \Psi^2(-x) \Rightarrow \\ &\Psi(x) = \pm\Psi(-x) \end{aligned}}$$

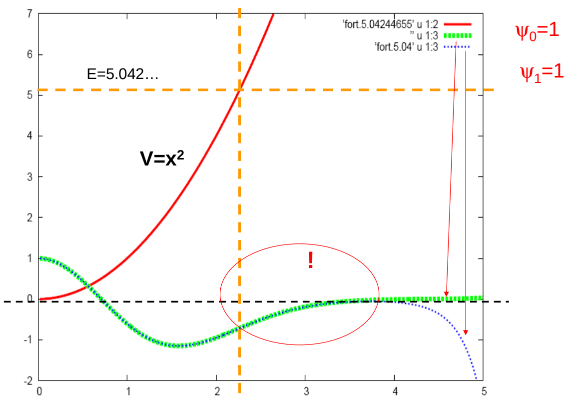
Luego son pares o impares

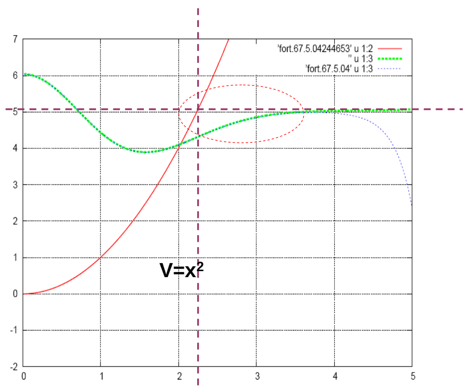
Si ahora me fijo en las pares en x=0

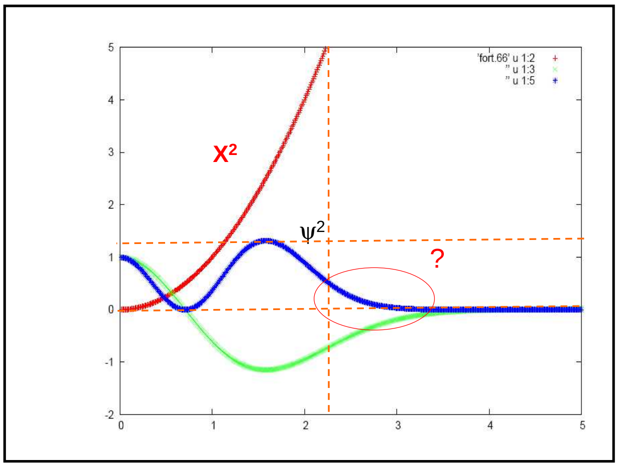
$$\psi_{j+1} = \left(2 - 2(\Delta z)^2\left[e - W_j\right]\right)\psi_j - \psi_{j-1}$$







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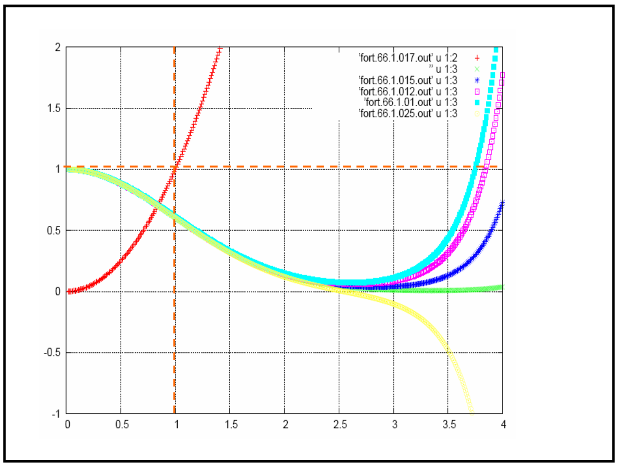
'' u 1:5
X^2
ψ^2
?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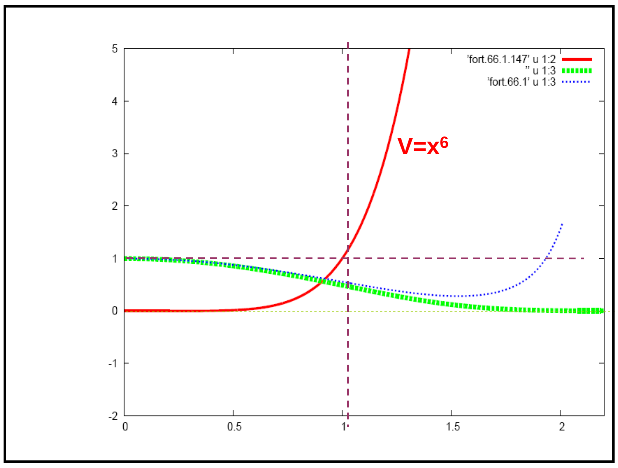
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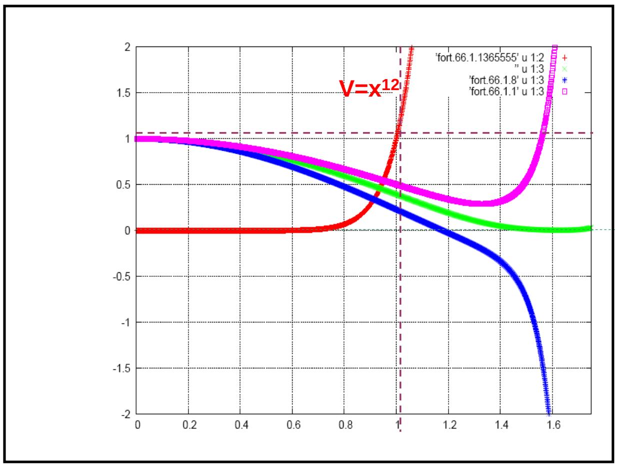
$V=x^6$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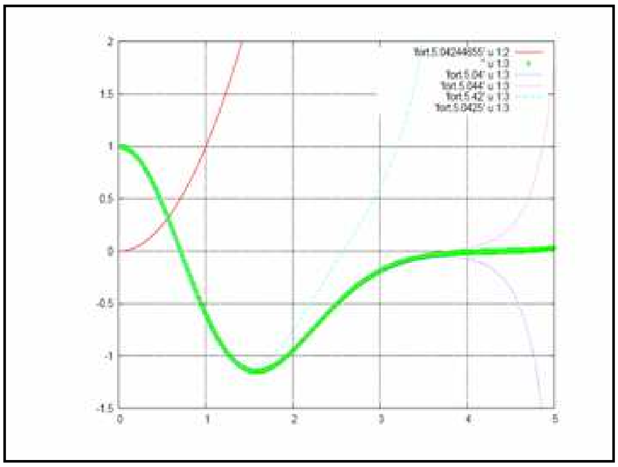
$V=x^{12}$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0
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-1
-1.5
0
1
2
3
4
5