Perturbation theory – basics

Read McIntyre 10.1-10.2

PH451/551

Recap $\left|\psi(t)\right\rangle = e^{-i\omega t/2}\left[\frac{e^{-in\omega t}}{\sqrt{2}}\left|n\right\rangle + \frac{e^{-im\omega t}}{\sqrt{2}}\left|m\right\rangle\right]$

1. Time dependence of <x>:

$$\left\langle\psi\right|x\left|\psi\right\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left[\frac{e^{+in\omega t}}{\sqrt{2}}\left\langle n\right| + \frac{e^{+im\omega t}}{\sqrt{2}}\left\langle m\right|\right]\left(a^{\dagger}+a\right)\left[\frac{e^{-in\omega t}}{\sqrt{2}}\left|n\right\rangle + \frac{e^{-im\omega t}}{\sqrt{2}}\left|m\right\rangle\right]$$

$$= \sqrt{\frac{\hbar}{8m\omega}}\left[e^{+i(n-m)\omega t}\left\langle n\right|\left(a^{\dagger}+a\right)\left|m\right\rangle + e^{+i(m-n)\omega t}\left\langle m\right|\left(a^{\dagger}+a\right)\left|n\right\rangle\right]$$

$$= \sqrt{\frac{\hbar}{8m\omega}}\begin{bmatrix} e^{+i(n-m)\omega t}\left(\sqrt{m+1}\,\delta_{n,m+1} + \sqrt{m}\,\delta_{n,m-1}\right) \\ +e^{+i(m-n)\omega t}\left(\sqrt{n+1}\,\delta_{m,n+1} + \sqrt{n}\,\delta_{m,n-1}\right) \end{bmatrix}$$

$$= \sqrt{\frac{\hbar}{8m\omega}}\begin{bmatrix} \left(e^{+i\omega t}\sqrt{n} + e^{-i\omega t}\sqrt{n+1}\right) \\ +\left(e^{+i\omega t}\sqrt{n+1} + e^{-i\omega t}\sqrt{n}\right) \end{bmatrix}$$

Recap $\left|\psi(t)\right\rangle = e^{-i\omega t/2}\left[\frac{e^{-in\omega t}}{\sqrt{2}}\left|n\right\rangle + \frac{e^{-im\omega t}}{\sqrt{2}}\left|m\right\rangle\right]$

1. Time dependence of <x>:

$$\left\langle\psi\right|x\left|\psi\right\rangle = \sqrt{\frac{\hbar}{8m\omega}}\left[\left(e^{+i\omega t} + e^{-i\omega t}\right)\sqrt{n} + \left(e^{+i\omega t} + e^{-i\omega t}\right)\sqrt{n+1}\right]$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\left[\sqrt{n} + \sqrt{n+1}\right]\cos\omega t$$

2. Radiation at freq omega!

3. Selection rule:

$$n - m = \pm 1$$

Reading Quiz

1. Write the Hamiltonian *H* of spin ½ electron in a magnetic field in the *z* direction (in the S_z basis):

2. Write the Hamiltonian *H* of spin ½ electron in a magnetic field that has components in the z direction and the *x*-direction (in the S_z basis):

Reading Quiz

1. Write the Hamiltonian *H* of spin ½ electron in a magnetic field in the *z* direction (in the S_z basis):

$$H = -\vec{\mu} \bullet \vec{B} = \frac{e}{2m} g\vec{S} \bullet \vec{B} = \frac{e}{2m} g S_z B_z$$

2. Write the Hamiltonian *H* of spin ½ electron in a magnetic field that has components in the *z* direction and the *x*-direction (in the S_z basis):

$$H = -\vec{\mu} \bullet \vec{B} = \frac{e}{2m} g\left(S_z B_z + S_x B_x\right)$$

Exact solutions – spin 1/2

1. Hamiltonian H: $$H = -\vec{\mu} \bullet \vec{B} = \frac{e}{2m} g \vec{S} \bullet \vec{B}$$
2. Large *B* in *z* direction (0^{th} order Hamiltonian H_0):

$$H_0 = \frac{e}{2m} g S_z B_{0(z)} = \omega_0 S_z = \frac{\hbar}{2} \begin{pmatrix} \omega_0 & 0 \\ 0 & -\omega_0 \end{pmatrix}$$

3. Add small *B* in z (perturbation Hamiltonian H'):

$$H = \frac{e}{2m} g S_z \left[B_{0(z)} + B_{1(z)} \right] = H_0 + H' =$$

$$= (\omega_0 + \omega_1) S_z = \frac{\hbar}{2} \begin{pmatrix} \omega_0 + \omega_1 & 0 \\ 0 & -\omega_0 - \omega_1 \end{pmatrix}$$

Exact solutions – spin 1/2

4. Add small B in *z* and *x* (perturbation Hamiltonian H'): (McI 2.1.2)

$$H = \frac{e}{2m} g \left\{ S_z \left[B_{0(z)} + B_{1(z)} \right] + S_x B_{2(x)} \right\} = H_0 + H' =$$

$$= \frac{\hbar}{2} \begin{pmatrix} \omega_0 + \omega_1 & \omega_2 \\ \omega_2 & -\omega_0 - \omega_1 \end{pmatrix}$$

5. Eigenvalues? (do for homework)

$$E_+ = \frac{\hbar}{2} \sqrt{\left(\omega_0 + \omega_1\right)^2 + \omega_2^2}$$

$$E_- = -\frac{\hbar}{2} \sqrt{\left(\omega_0 + \omega_1\right)^2 + \omega_2^2}$$

Approx solutions – spin 1/2

1. IF we assume perturbation is small, then ....

$$E_{\pm} \cong \pm\left[\frac{\hbar\omega_0}{2} + \frac{\hbar\omega_1}{2} + \frac{\hbar\omega_2^2}{4\omega_0}\right]$$

0th order energy $E^{(0)}$

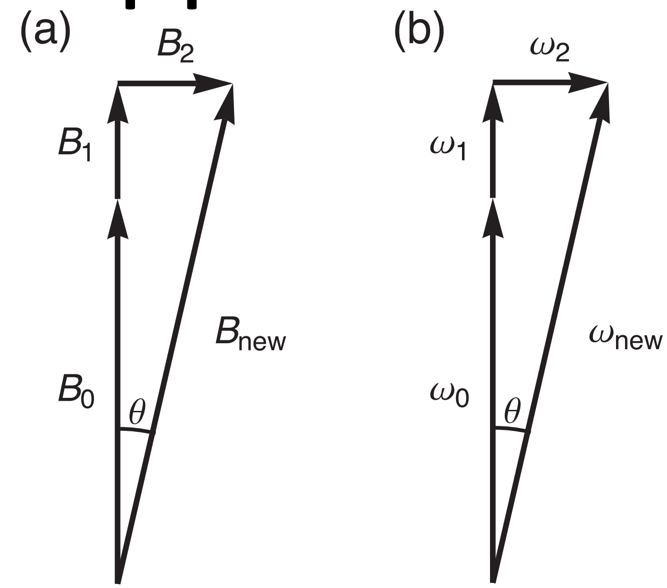
1st order correction $E^{(1)}$

2nd order correction $E^{(2)}$

$$H_0 = \begin{pmatrix} \frac{\hbar\omega_0}{2} & 0 \\ 0 & -\frac{\hbar\omega_0}{2} \end{pmatrix}$$

$$H' = \begin{pmatrix} \frac{\hbar\omega_1}{2} & \frac{\hbar\omega_2}{2} \\ \frac{\hbar\omega_2}{2} & -\frac{\hbar\omega_1}{2} \end{pmatrix}$$

Eigenstates – exact & approx



1. Exact eigenstates (McI 2.2):

$$|+\rangle_n = \cos\frac{\theta}{2}|+\rangle + \sin\frac{\theta}{2}|-\rangle$$

$$|-\rangle_n = -\sin\frac{\theta}{2}|+\rangle + \cos\frac{\theta}{2}|-\rangle$$

2. IF we assume perturbation is small, then …

$$|+\rangle_n \cong |+\rangle + \frac{\theta}{2}|-\rangle = |+\rangle + \frac{\omega_2}{2\omega_0}|-\rangle$$

$$|-\rangle_n \cong |-\rangle - \frac{\theta}{2}|+\rangle = |-\rangle - \frac{\omega_2}{2\omega_0}|+\rangle$$

1st order correction from orthog state

$$H' = \begin{pmatrix} \frac{\hbar\omega_1}{2} & \frac{\hbar\omega_2}{2} \\ \frac{\hbar\omega_2}{2} & -\frac{\hbar\omega_1}{2} \end{pmatrix}$$

spin ½ in B_z + little B_z

$$H_0 = \frac{\hbar}{2}\begin{pmatrix} \omega_0 & 0 \\ 0 & -\omega_0 \end{pmatrix}$$

$$H' = \frac{\hbar}{2}\begin{pmatrix} \omega_1 & 0 \\ 0 & -\omega_1 \end{pmatrix}$$

spin ½ in B_z + little B_x

$$H_0 = \frac{\hbar}{2}\begin{pmatrix} \omega_0 & 0 \\ 0 & -\omega_0 \end{pmatrix}$$

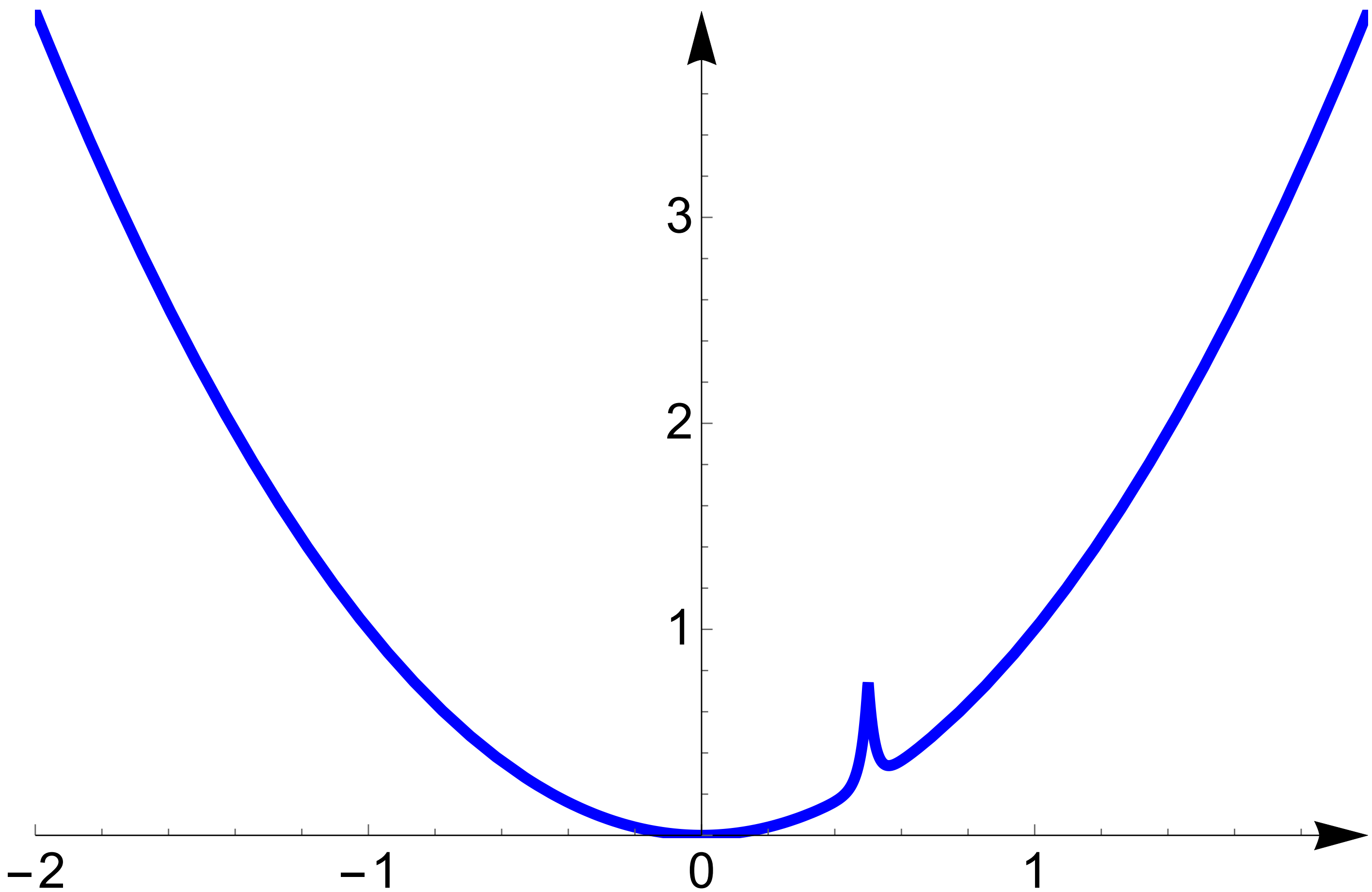
$$H' = \frac{\hbar}{2}\begin{pmatrix} 0 & \omega_2 \\ \omega_2 & 0 \end{pmatrix}$$

spin ½ in B_z + little B_x

$$H_0 = \frac{\hbar}{2}\begin{pmatrix} \omega_0 & 0 \\ 0 & -\omega_0 \end{pmatrix}$$

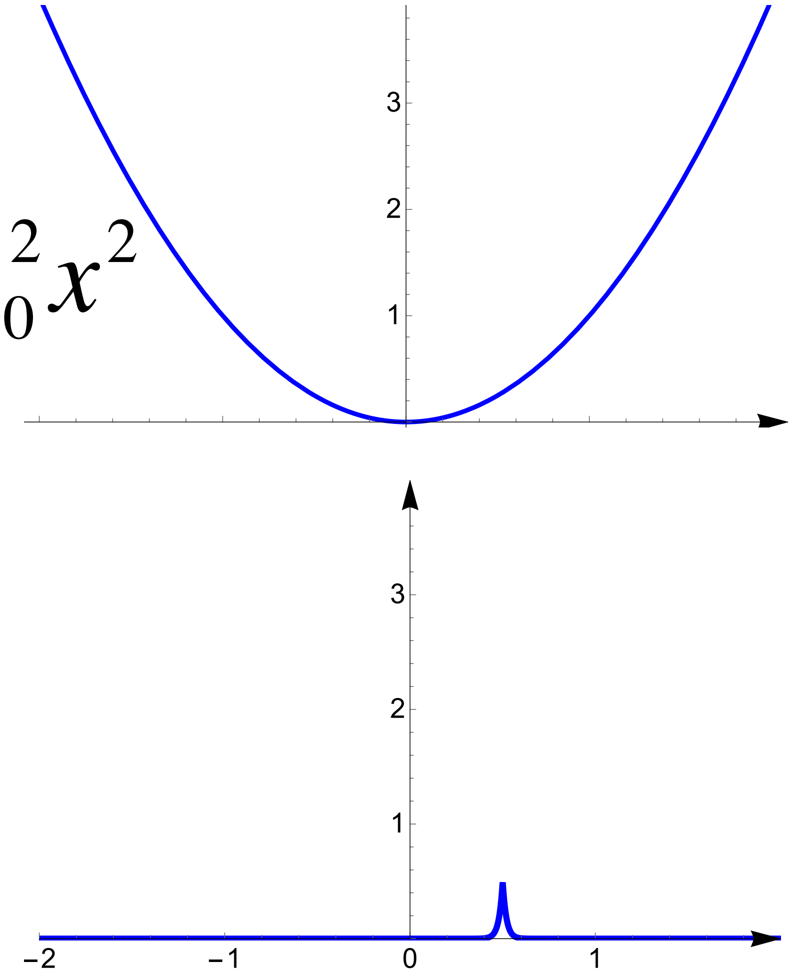
$$H' = \frac{\hbar}{2}\begin{pmatrix} 0 & \omega_2 \\ \omega_2 & 0 \end{pmatrix}$$

Harmonic Oscillator + perturbation



Harmonic Oscillator + perturbation

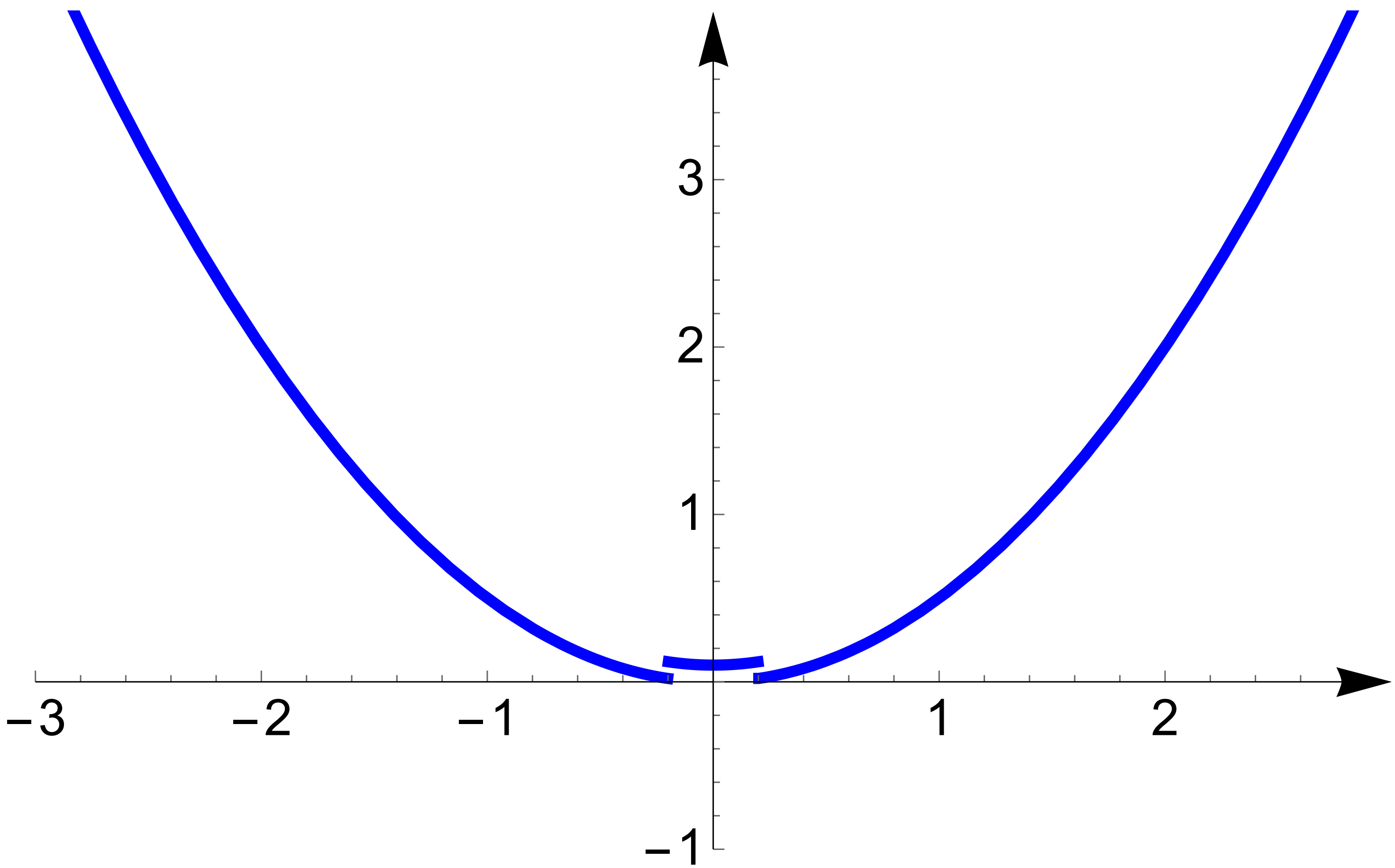
$$H_0 = \frac{p^2}{2m} + \frac{1}{2} m\omega_0^2 x^2$$



$$H' = \varepsilon e^{-|x-x_0|/d}$$

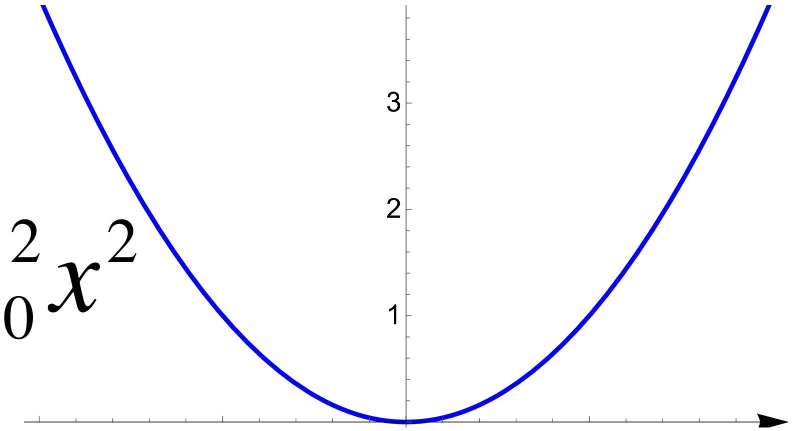
$$\varepsilon << \frac{\hbar\omega_0}{2}$$

Harmonic Oscillator + perturbation



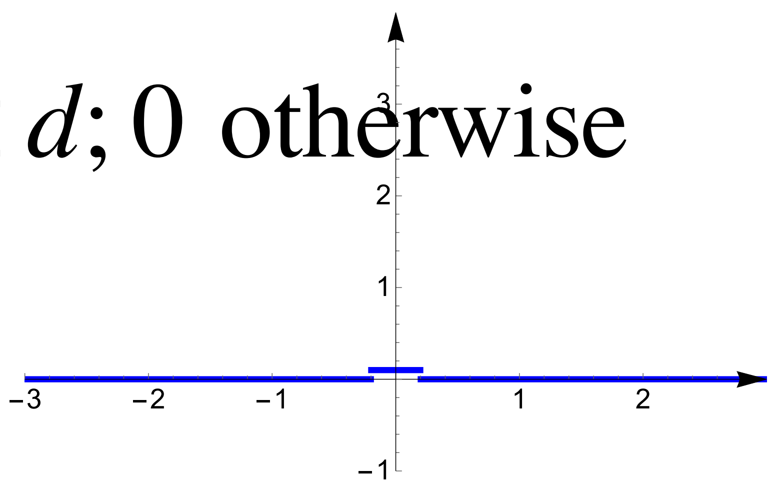
Harmonic Oscillator + perturbation

$$H_0 = \frac{p^2}{2m} + \frac{1}{2} m \omega_0^2 x^2$$



$$H' = \varepsilon \quad -d < x < d; 0 \text{ otherwise}$$

$$\varepsilon << \frac{\hbar \omega_0}{2}$$



Harmonic Oscillator + perturbation

$$H_0 = \hbar\omega_0 \begin{pmatrix} 1/2 & 0 & 0 & 0 \\ 0 & 3/2 & 0 & 0 \\ 0 & 0 & n+1/2 & 0 \\ 0 & 0 & 0 & \ldots \end{pmatrix}$$

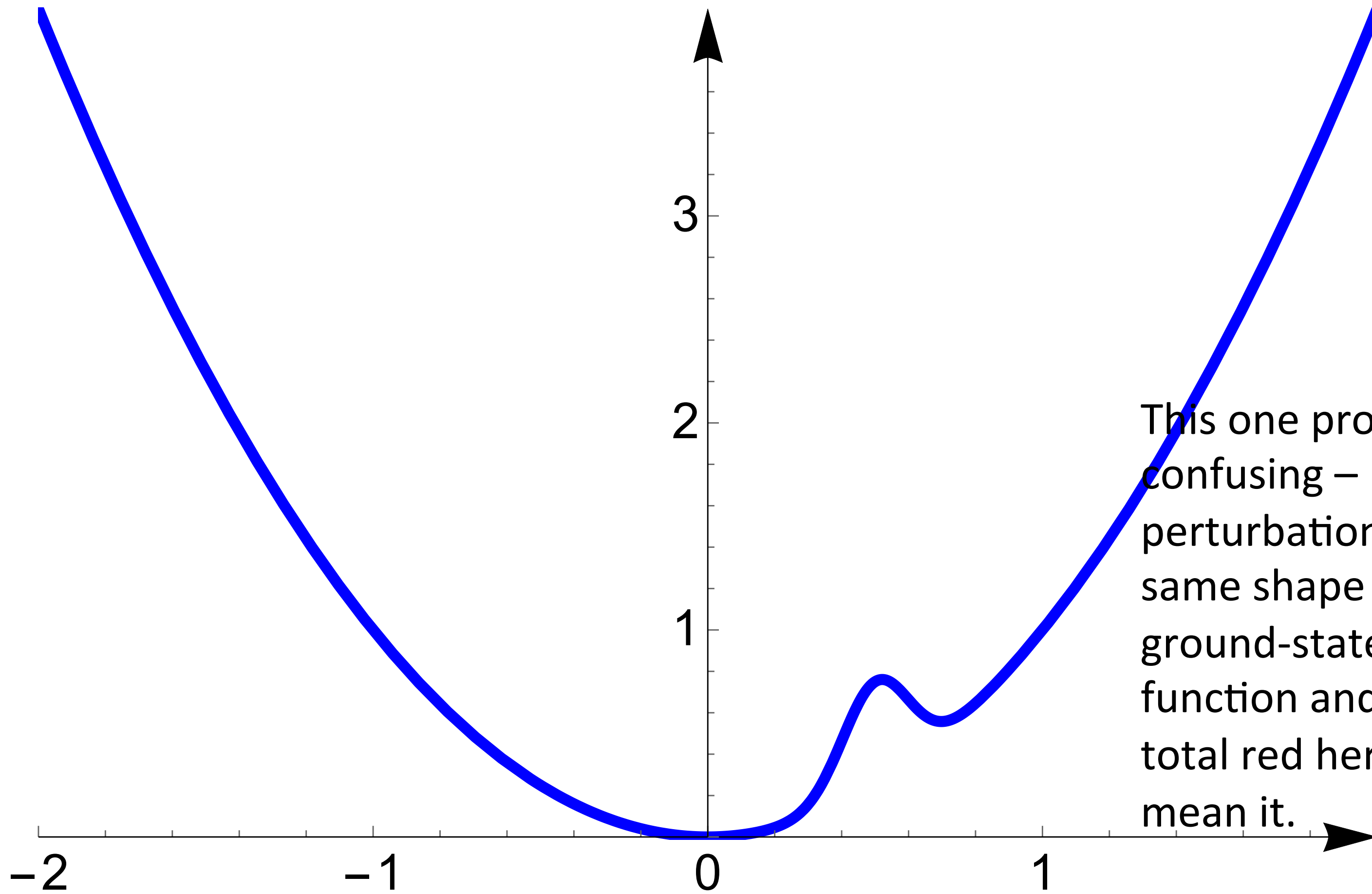
$$H' = ???$$

Harmonic Oscillator + perturbation

$$H_0 = \hbar\omega_0 \begin{pmatrix} 1/2 & 0 & 0 & 0 \\ 0 & 3/2 & 0 & 0 \\ 0 & 0 & n+1/2 & 0 \\ 0 & 0 & 0 & \ldots \end{pmatrix}$$

$$H' = \hbar\omega_0 \begin{pmatrix} 0.0222703 & 0. & -0.015332 \\ 0. & 0.000587563 & 0. \\ -0.015332 & 0. & 0.0105616 \end{pmatrix}$$

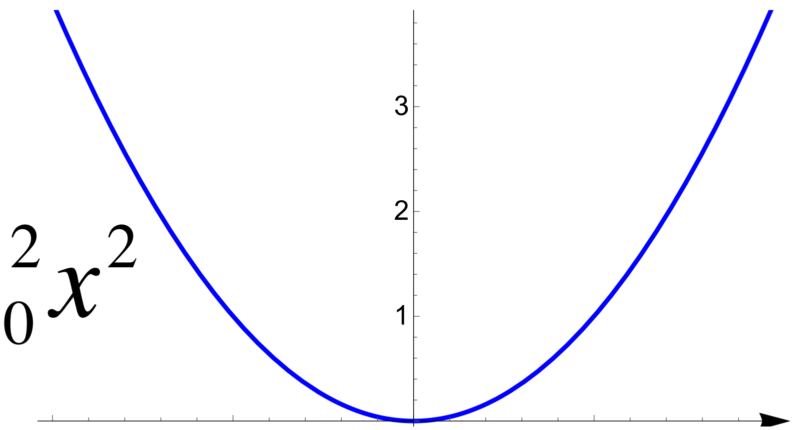
Harmonic Oscillator + different perturbation



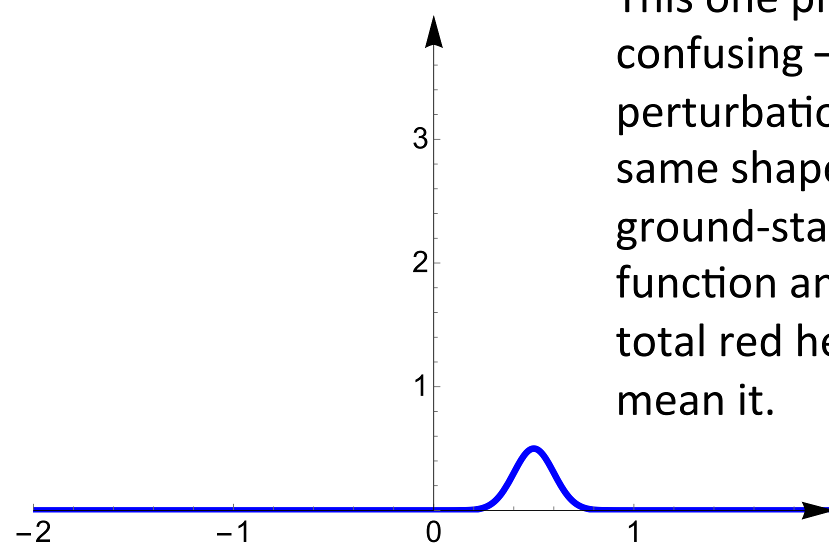
This one proved confusing – perturbation has the same shape as the ground-state wave function and that is a total red herring! Didn't mean it.

Harmonic Oscillator + different perturbation

$$H_0 = \frac{p^2}{2m} + \frac{1}{2} m\omega_0^2 x^2$$



$$H' = \varepsilon e^{-(x-x_0)^2/d}$$



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