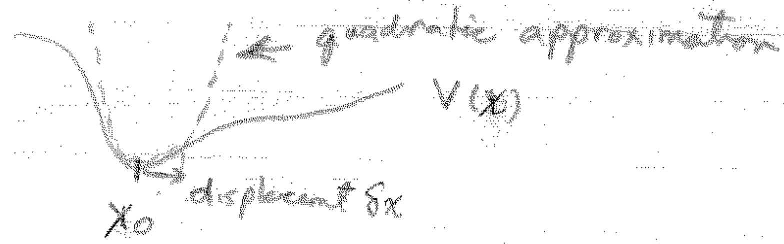
Physics 491: Quantum Mechanics I
Problem Set #9: Solutions

Problem 1: Physical example of harmonics oscillators

Consider a potential which has a stable equilibrium point



The quadratic approximation follows from a Taylor series to $V(x)$ around the equilibrium.

The equilibrium point is the minimum of the potential defined by $\left.\frac{dV}{dx}\right|_{x_0} = 0$ with $\left.\frac{d^2V}{dx^2}\right|_{x_0} > 0$

To second order:

$$V(x) = V(x_0) + \frac{1}{2}\left.\frac{d^2V}{dx^2}\right|_{x_0}(x-x_0)^2$$

$$= V_0 + \frac{1}{2}k(\delta x)^2$$

where $k = \left.\frac{d^2V}{dx^2}\right|_{x_0} = V_0''$ is the "spring constant"

$\Rightarrow$ Oscillation frequency $\omega = \sqrt{\frac{k}{m}} = \sqrt{\frac{V_0''}{m}}$

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Of course, the quadratic approximation breaks down when the displacement δx gets large enough

$$V(x) = V_0 + \frac{1}{2} V_0''(x-x_0)^2 + \frac{1}{3!} V_0'''(x-x_0)^3 + \frac{1}{4!} V_0''''(x-x_0)^4 + \dots$$

When $\delta x = x - x_0$ gets large enough the higher order terms begin to dominate and the infinite series doesn't converge. this sets a "nonlinear scale" for the potential.

Thus for example, if the cubic term is nonvanishing we can define a "nonlinear scale" as the displace ~~that is~~ term is on order the quadratic

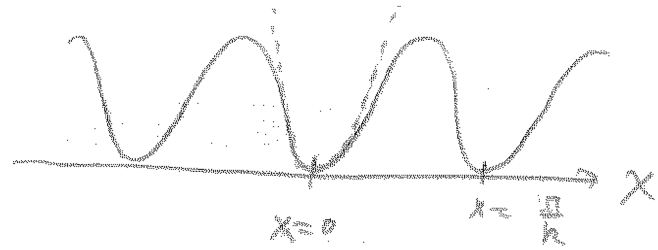
i.e. $$\left| \frac{1}{2} V_0'' (\delta x_{NL})^2 \right| = \left| \frac{1}{6} V_0''' (\delta x_{NL})^3 \right|$$

$$\Rightarrow \quad \delta x_{NL} = \left| 3 \frac{V_0''}{V_0'''} \right|$$

So, when is it reasonable to quantize the potential as a SHO? Clearly we must have the zero point motion $\ll \delta x_{NL}$. Otherwise the wave packet never "experiences" a harmonic potential.

$$\Rightarrow \quad \Delta x_0 = \sqrt{\frac{\hbar}{2m\omega}} \ll \delta x_{NL}$$

(a) Periodic potential $V(x) = V_0 \sin^2 kx$



Multiple equilibria. We can pick any of them (they are equivalent)

Expanding around $x=0$, $\sin kx \approx kx + \frac{1}{6}(kx)^3$

$$\Rightarrow V(x) \approx V_0 \left(k^2 x^2 + \frac{1}{3}(kx)^4 + \cdots\right)$$

Quadratic approximation $V(x) \approx V_0 k^2 x^2 = \frac{1}{2} m\omega^2 x^2$

$$\Rightarrow \omega = \sqrt{2V_0 k^2/m} \Rightarrow \Delta X_0 = \sqrt{\frac{\hbar}{2m\omega}} =$$

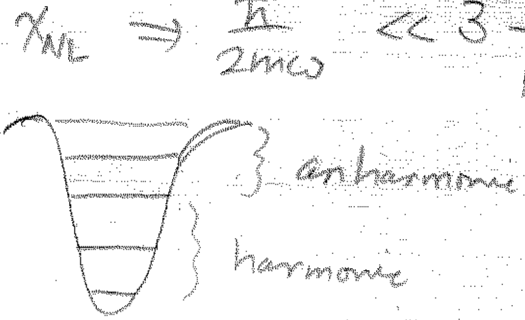
Nonlinear scale – when quartic term becomes important

$$\Rightarrow \text{When } k^2 x_{NL}^2 \approx \frac{1}{3} k^4 x_{NL}^4$$

$$\Rightarrow x_{NL} = \sqrt{3}\,\frac{1}{k}$$

The SHO applies if $\Delta X_0 \ll x_{NL} \Rightarrow \frac{\hbar}{2m\omega} \ll 3\frac{1}{k^2}$

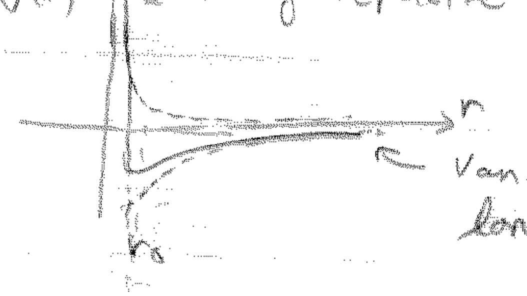
$$\Rightarrow \boxed{V_0 \gg \frac{1}{72}\frac{\hbar^2 k^2}{m}}$$



For some choice

(b) Leonard-Jones $V(r) = \frac{C_{12}}{r^{12}} - \frac{C_6}{r^6}$

The "phenomenological potential" was invented to characterize the binding of atoms into molecules.



Equilibrium separation: $\left.\frac{dV}{dr}\right|_{r_0} = \frac{-12C_{12}}{r_0^{13}} + \frac{6C_6}{r_0^7} = 0$

$$\Rightarrow r_0 = \left(\frac{2C_{12}}{C_6}\right)^{1/6}$$

Taylor Series: $V(r) = V(r_0) + \frac{1}{2}V_0''(r-r_0)^2 + \frac{1}{6}V_0'''(r-r_0)^3$

Oscillation frequency for small displacements

$$\omega = \sqrt{\frac{V_0''}{m}}$$

Let $x = r - r_0$ = displacement from origin

Nonlinear scale: $\left|\frac{1}{2}V_0'' x_{NL}^2\right| = \left|\frac{1}{6}V_0''' x_{NL}^3\right|$

$$\Rightarrow x_{NL} = \left|\frac{3V_0''}{V_0'''}\right|$$

Quantum oscillator good approximation when

$$x_{NL} << \sqrt{\frac{\hbar}{2m\omega}} \Rightarrow \hbar\omega << \frac{\hbar^2}{2m x_{NL}^2}$$

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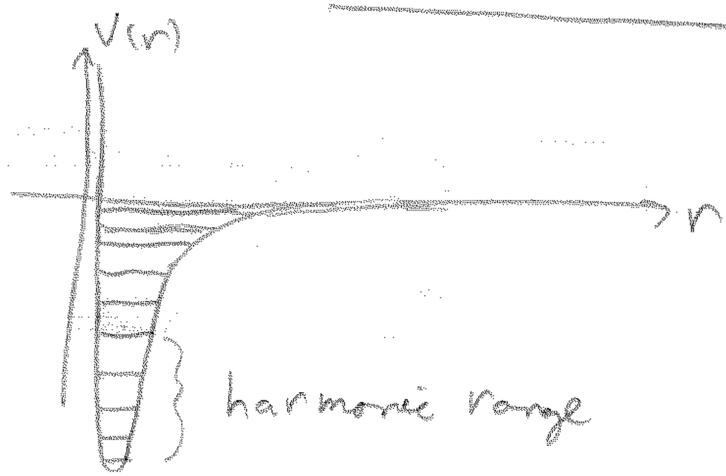
$$\sqrt{\frac{V_0''}{m}} \ll \frac{\hbar}{18m}\left(\frac{V_0'''}{V_0''}\right)^2$$

$$\Rightarrow \frac{(V_0'')^5}{(V_0''')^4} \ll \frac{\hbar^2}{324\, m}$$

$\Rightarrow$ Require $\boxed{\frac{C_6^5}{C_{12}^2} \ll 1.85\times10^3 \,\frac{\hbar^6}{m^3}}$



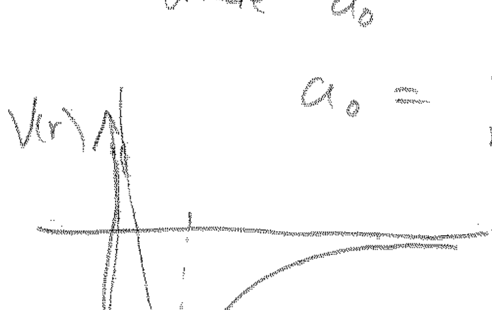
For some choice of parameters

(c) p-state in Hydrogenic atom

$$V(r) = \frac{\hbar^2}{mr^2} - \frac{e^2}{r} = E_0\left(\frac{a_0^2}{r^2} - \frac{a_0}{r}\right)$$

where $\frac{e^2}{a_0} = \frac{me^4}{\hbar^2}$ = Hartree

$a_0 = \frac{\hbar^2}{me^2}$ = Bohr radius



$$\left.\frac{dV}{dr}\right|_{r_0} = E_0\left(-\frac{2a_0^2}{r_0^3} + \frac{a_0}{r_0^2}\right) = 0$$

$$\Rightarrow r_0 = 2a_0$$

Taylor series:

$$V(r) = V_0 + \frac{1}{2} V_0''(r-r_0)^2 + \frac{1}{6} V_0'''(r-r_0)^3 + \dots$$

$$V_0'' = \frac{d^2V}{dr^2}\bigg|_{r_0} = \frac{E_0}{8} \frac{1}{a_0^2}$$

$$V_0''' = \frac{d^3V}{dr^3}\bigg|_{r_0} = -\frac{3E_0}{8} \frac{1}{a_0^3}$$

Harmonic approximation when

$$\Delta x_0 \ll x_{NL} \quad \text{or} \quad \hbar\omega \ll \frac{\hbar^2}{2m x_{NL}^2}$$

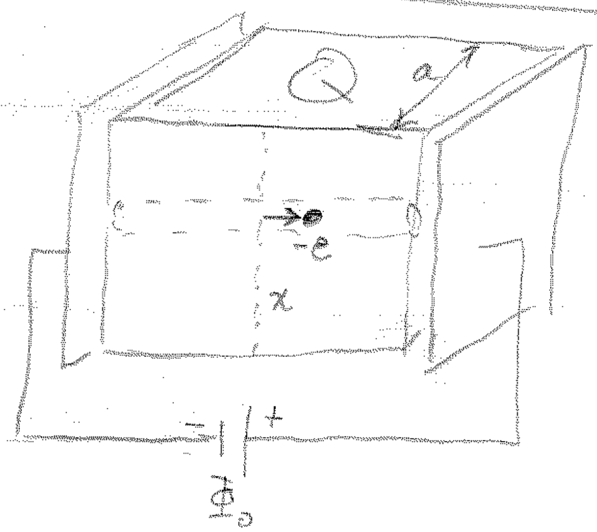
We solved this in part (b)

$$\Rightarrow \text{Require} \quad \frac{(V_0'')^5}{(V_0''')^4} \ll \frac{\hbar^2}{324 m} \Rightarrow \frac{\left(\frac{E_0}{8} \frac{1}{a_0^2}\right)^5}{\left(\frac{3}{8} E_0 \frac{1}{a_0^3}\right)^4} \ll \frac{\hbar^2}{324 m}$$

$$\frac{1}{72} E_0 \ll \frac{\hbar^2}{324\, m a_0^2} = \frac{1}{324} E_0$$

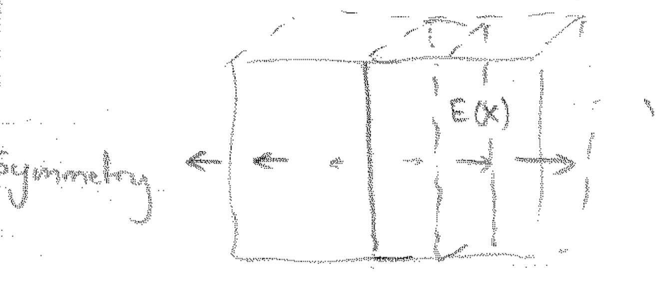
$\boxed{\text{Impossible}}$! The energy levels of $l=1$ Hydrogen are not harmonic. They are not equally spaced in any range.

Problem 2:



Electron moving in 1D inside a uniformly charged cube superimposed on the field inside a capacitor with potential difference Φ_0

If we ignore fringing fields, then near the center of the cube the electric field is in the x-direction. Use Gauss' Law to find the field due to the cube



E = 0 at center

$$\oint \vec{E} \cdot d\vec{a} = \underbrace{\left[\frac{1}{4\pi\epsilon_0}\right]}_{=1 \text{ in cgs}} 4\pi Q_{enc}$$

Ignoring fringing fields, flux is non-zero only on surface at x

$$\Rightarrow \oint \vec{E} \cdot d\vec{a} = E(x)\, A = \left[\frac{1}{4\pi\epsilon_0}\right] 4\pi \frac{Q}{L^3} (A x)$$

$$\Rightarrow E(x) = \left[\frac{1}{4\pi\epsilon_0}\right] \frac{4\pi Q}{L^3} x$$

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thus the potential energy of the electron due the the field of the cube

$$V_{cube}(x) = -(-e)x\,E(x) = \left[\frac{1}{4\pi\epsilon_0}\right]\left(+\frac{4\pi eQ}{L^3}\right)x^2$$

$\uparrow$ electron charge

the electric field due to the capacitor is uniform

$$E_{capacitor} = -\Phi_0/L$$

$$\Rightarrow V_{cap}(x) = -(-e)\,x\,E(x) = -\frac{e\Phi_0}{L}x$$

$$\Rightarrow \text{Hamilton} \quad \hat{H} = \frac{\hat{p}^2}{2m} + V_{cube}(\hat{x}) + V_{cap}(\hat{x})$$

$$\boxed{\hat{H} = \frac{\hat{p}^2}{2m} + \left[\frac{1}{4\pi\epsilon_0}\right]\left(\frac{4\pi eQ}{L^3}\right)x^2 - \frac{e\Phi_0}{L}x}$$

(a) Harmonic potential with spring constant

$$\boxed{K = \left[\frac{1}{4\pi\epsilon_0}\right]\frac{8\pi eQ}{L^3}}$$

(b) The capacitor acts to displace the equilibrium point. The potential energy for displacements around this new equilibrium point is still harmonic

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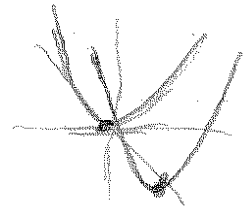
Generally : Given $V(x) = \frac{1}{2} K x^2 + a x$



← displaced oscillator

Complete the square

$$V(x) = \frac{1}{2} K \left(x + \frac{a}{K}\right)^2 - \frac{1}{2} \frac{a}{K^2}$$

Thus

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} K (\hat{x} - x_0)^2 + C$$

where $K = \left[\frac{1}{4\pi\epsilon_0}\right] \left(\frac{4\pi e Q}{L^3}\right) x^2$

$$x_0 = \frac{e\Phi_0}{LK}, \qquad C = -\frac{1}{2} \frac{x_0}{K^2}$$

The energy levels are then just those of the SHO, shifted by the constant C

$$\boxed{E_n = \hbar\omega\left(n + \frac{1}{2}\right) + C \qquad \omega = \sqrt{\frac{K}{m}}}$$

Problem 3

The n^{th} excited state of the harmonic oscillator

$$|n\rangle = \frac{1}{\sqrt{n!}}(\hat{a}^{+})^{n}\,|0\rangle$$

Given $\langle 0|0\rangle = 1$ show $\langle n|n\rangle = 1$

Proof: $\langle n|n\rangle = \frac{1}{n!}\langle 0|\hat{a}^{n}(\hat{a}^{+})^{n}|0\rangle$

Aside: $\hat{a}|0\rangle = 0 \Rightarrow \hat{a}^{n}|0\rangle = 0$

$$\therefore\ \langle n|n\rangle = \frac{1}{n!}\langle 0|[\hat{a}^{n},(\hat{a}^{+})^{n}]\,|0\rangle$$

Aside: $[\hat{a}^{n},(\hat{a}^{+})^{n}] = \hat{a}^{n-1}[\hat{a},(\hat{a}^{+})^{n}] + [\hat{a}^{n-1},\hat{a}^{+n}]\hat{a}$

$$\Rightarrow \langle n|n\rangle = \frac{1}{n!}\langle 0|\hat{a}^{n-1}[\hat{a},(\hat{a}^{+})^{n}]\,|0\rangle$$

Aside: $[\hat{a},(\hat{a}^{+})^{n}] = (\hat{a}^{+})^{n-1}\underbrace{[\hat{a},\hat{a}^{+}]}_{=1} + [\hat{a},(\hat{a}^{+})^{n-1}]\,\hat{a}^{+}$

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$$[\hat{a}, (\hat{a}^{+})^{n}] = (\hat{a}^{+})^{n-1} + [\hat{a}, (\hat{a}^{+})^{n-1}]\hat{a}^{+}$$

Recursively, $[\hat{a}, (\hat{a}^{+})^{n}] = n(\hat{a}^{+})^{n-1}$

$$\Rightarrow \langle 0|\hat{a}^{n}(\hat{a}^{+})^{n}|0\rangle = n\langle 0|(\hat{a})^{n-1}(\hat{a}^{+})^{n-1}|0\rangle$$

Thus recursively $\langle 0|\hat{a}^{n}(\hat{a}^{+})^{n}|0\rangle = n!$

$$\Rightarrow \langle n|n\rangle = 1$$

(c) $\hat{A}$ is a "positive operator"

$$\Rightarrow \forall |\psi\rangle \qquad \langle\psi|\hat{A}|\psi\rangle \geq 0$$

Let $|\psi\rangle = |a\rangle$ (an eigenvector of $\hat{A}$)

$$\Rightarrow \langle a|\hat{A}|a\rangle = a \geq 0 \qquad \text{q.e.d.}$$

(d) The n^{th} excited state of the harmonic oscillator

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Aside: $[\hat{a}^{n},(\hat{a}^{+})^{n}] = \hat{a}^{n-1}[\hat{a},(\hat{a}^{+})^{n}] + [\hat{a}^{n-1},\hat{a}^{+n}]\hat{a}$

$$\Rightarrow \langle n|n\rangle = \frac{1}{n!}\langle 0|\hat{a}^{n-1}[\hat{a},(\hat{a}^{+})^{n}]|0\rangle$$

Aside: $[\hat{a},(\hat{a}^{+})^{n}] = (\hat{a}^{+})^{n-1}\underbrace{[\hat{a},\hat{a}^{+}]}_{=1} + [\hat{a},(\hat{a}^{+})^{n-1}]\hat{a}^{+}$

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