

Physics 492 - Quantum II

Problem Set #2 - Solutions

Problem 1:

(a) If $\hat{C} = \hat{A}\hat{B}$, show $\hat{C}^\dagger = \hat{B}^\dagger\hat{A}^\dagger$

Proof. Let $|\phi\rangle = \hat{C}|\psi\rangle \Rightarrow \langle\phi| = \langle\psi|\hat{C}^\dagger$

But $\hat{C}|\psi\rangle = \hat{A}\hat{B}|\psi\rangle = \hat{A}|\chi\rangle$
Define $|\chi\rangle$

$$\Rightarrow \langle\phi|\hat{C}^\dagger = \langle\chi|\hat{A}^\dagger = \langle\psi|\hat{B}^\dagger\hat{A}^\dagger$$

q.e.d.

(b) $\hat{A}|a\rangle = a|a\rangle$ Hermitian operator

State $|\psi\rangle \Rightarrow P_a = |\langle a|\psi\rangle|^2$

$$\langle A \rangle = \sum_a a P_a = \sum_a a |\langle a|\psi\rangle|^2$$

$$= \sum_a a \langle\psi|a\rangle\langle a|\psi\rangle$$

$$= \langle\psi| \underbrace{\left(\sum_a a |a\rangle\langle a|\right)}_{=\hat{A}} |\psi\rangle$$

$$\Rightarrow \langle A \rangle = \langle\psi|\hat{A}|\psi\rangle \quad \text{q.e.d.}$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

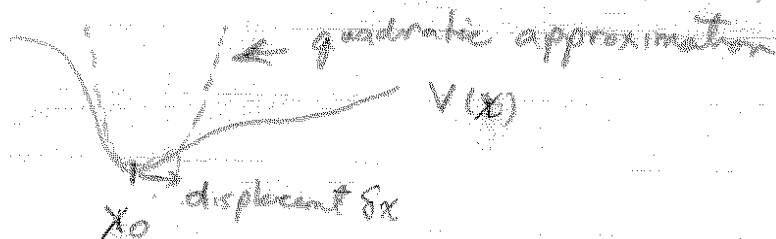
$$\Rightarrow \langle 0 | \hat{a}^n (\hat{a}^\dagger)^n | 0 \rangle = n \langle 0 | \hat{a}^{n-1} (\hat{a}^\dagger)^{n-1} | 0 \rangle$$

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

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

Problem 2: Physical example of harmonic 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 $\frac{dV}{dx}|_{x_0} = 0$ with $\frac{d^2V}{dx^2}|_{x_0} > 0$

To second order:

$$V(x) = V(x_0) + \frac{1}{2} \frac{d^2V}{dx^2}|_{x_0} (x-x_0)^2$$
$$= V_0 + \frac{1}{2} k (\delta x)^2$$

where $k = \frac{d^2V}{dx^2}|_{x_0} = V''_0$ is the "spring constant"

⇒ 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

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

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 displacement that is term is on order the quadratic

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

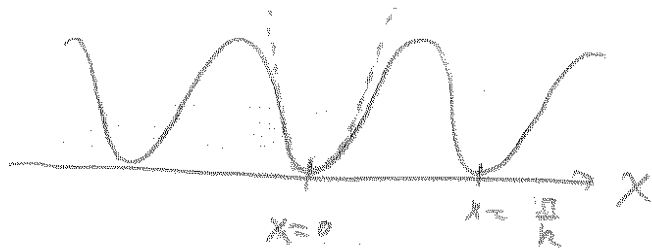
$$\Rightarrow \delta x_{NL} = \left| 3 \frac{V_0''}{V_0'''} \right|$$

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.

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

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



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

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

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

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

$$\Rightarrow \omega = \sqrt{2V_0 k^2 / m} \Rightarrow \Delta x_0 = \sqrt{\frac{\hbar}{2m\omega}} =$$

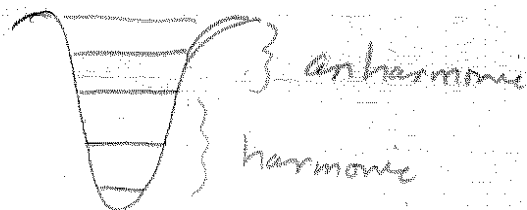
Nonlinear scale - when quartic term becomes important

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

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

The SHO applies if $\Delta x_0 \ll x_{NL} \Rightarrow \frac{\hbar}{2m\omega} \ll 3 \frac{1}{k^2}$

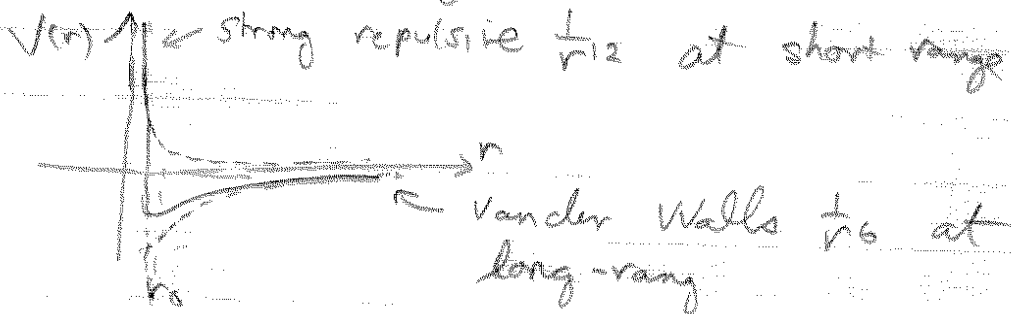
$$\Rightarrow \boxed{V_0 \gg \frac{1}{72} \frac{\hbar^2 k^2}{m}}$$



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: $\frac{dV}{dr}\bigg|_{r_0} = -\frac{12C_{12}}{r_0^{13}} + \frac{6C_6}{r_0^7} = 0$

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

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

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

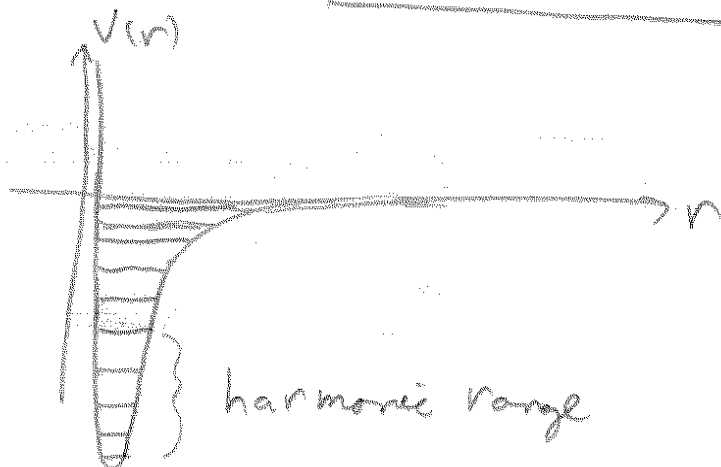
Quantum oscillator good approximation when

$$x_{NL} \ll \sqrt{\frac{\hbar}{2m\omega}} \Rightarrow \hbar\omega \ll \frac{\hbar^2}{2m x_{NL}^2} \quad (\text{Next Page})$$

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

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

$$\Rightarrow \text{Require } \frac{C_6^5}{C_{12}^2} \ll 1.85 \times 10^3 \frac{\hbar^6}{m^3}$$



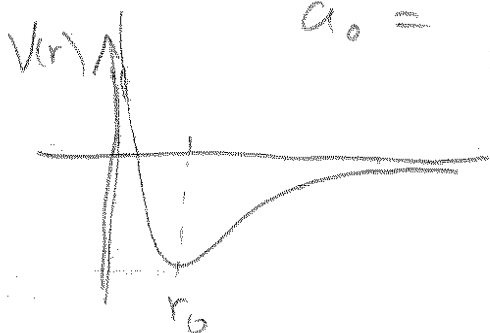
For some choice of parameters

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

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



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

$$\Rightarrow r_0 = 2a_0$$

Taylor series:

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

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

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

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)

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

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

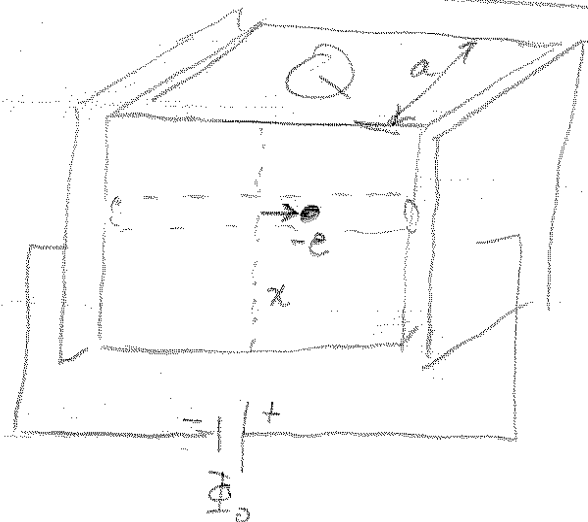
Impossible ! The energy levels

of $l=1$ Hydrogen are not harmonic.

They are not equally spaced in

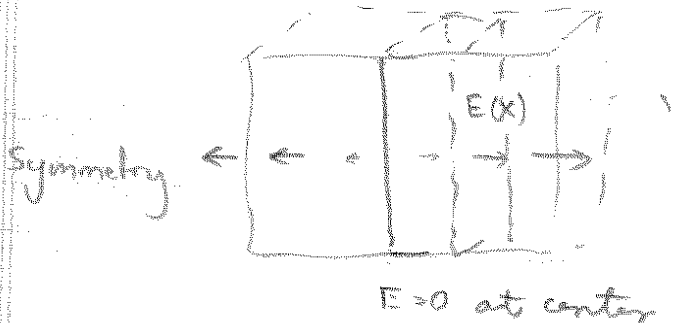
any range.

Problem 3: Liboff 7.16



Electrons 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.



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

$= 1$ in cgs

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

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

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

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Thus the potential energy of the electron due to the field of the cube

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

↑
electron charge

The electric field due to the capacitor is uniform

$$E_{\text{capacitor}} = -\frac{\Phi_0}{L}$$

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

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

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

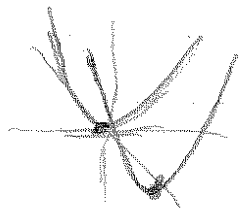
(a) Harmonic potential with spring constant

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

(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 $V(x) = \frac{1}{2}Kx^2 + ax$



← displaced oscillator

Complete the square

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

Thus

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

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

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

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

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

$$\omega = \sqrt{\frac{K}{m}}$$