PHYS 4410

Quantum Mechanics 2

Spring 2023

Lecture 1

Harmonic oscillator: heuristic analysis

January 18

1

- Recorded via Zoom Canvas plug-in

Book/Notes: McIntyre / Tong

help? - class Slack (invite link on Canvas)
- OH: 8-9 PM Tues
2:30-3:30 PM Wed

grading: 40% HWS [10-12 total] due Thurs.
3 "extensions": drop/ignore / 48 hr late
60% exam [3 total, 2 hr in person]

2

Problem 2 (Covalent bond): An extremely important system that can be modeled accurately by a simple harmonic oscillator is the chemical bond in a diatomic molecule A_2, with A = H, N, F, O, etc. If the A atom has mass m, then the Hamiltonian describing the simple harmonic oscillator is

$$H = \frac{p^2}{m} + \frac{1}{4}m\omega^2x^2. \tag{5}$$

The funny constant factors above are deliberate, and arise because the harmonic oscillation describes the *relative motion* of the two atoms.

points 15 **A:** Let $|0\rangle$ denote the ground state of this oscillator. Evaluate the "size" D of this oscillator in the ground state, and show that

$$D = \sqrt{\langle 0|x^2|0\rangle} = \sqrt{\frac{\hbar}{m\omega}}. \tag{6}$$

A atom	m (10^{-27} kg)	ω (10^{12} Hz)	L (10^{-10} m)
H	1.7	827	0.7
N	23.4	438	1.1
Cl	58.5	104	2.0
Br	132	61	2.3

Figure 1: (Rough) experimental values of m, ω, and L for simple diatomic molecules.

10 **B:** The data in Figure 1 lists the experimentally determined bond length L of the covalent bond in the A_2 molecule. Is D or L larger? Does your answer make physical sense?

graded: 0, 2, 4, 6, 8, 10

HW + exams: graded out of 100, but ≥ 115 points

A / A- : ≥ 90% (or top 1/3)

B+/ B / B- : ≥ 75%

C+/C/C- : ≥ 60% (all?)

3

PISEC

Partnerships for Informal Science Education in the Community

ATTEND AN INFO SESSION

Thursday 1/19, 2-3pm, JILA X325

Friday 1/20, 10-11am, Zoom (tinyurl.com/PISECinfoZoom)

Monday 1/23, 12-1pm, JILA X325

SIGN UP HERE

tinyurl.com/PISECsignup-Sp23

- ★ Partner with K-12 students on fun physics experiments
- ★ Work with students underrepresented in STEM
- ★ Cultivate interest, support identity development, pathways into STEM
- ★ Gain teaching & science communication experience, build community

colorado.edu/outreach/pisec

Questions? Email Jessica.Hoehn@Colorado.edu

PISEC

$\boxed{4}$ interactions btwn (neutral) atoms (^4He)

fixed $\quad \xleftrightarrow{x} \quad$ mobile

He $\qquad\qquad$ He

$$V(x) = U\left[\left(\frac{a}{x}\right)^{12} - \left(\frac{a}{x}\right)^{6}\right]$$

van der Waals

empirical

binding: 10^{-23} J

10^{-10} m

from QM I:

$$\overbrace{-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}}^{\text{kinetic}} + \overbrace{V(x)\psi}^{\text{pot.}} = E\psi$$

Solve? [for E and/or ψ]. Impossible.

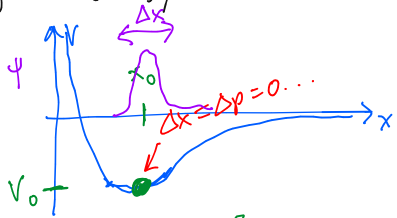
#1 ~~numerics~~

#2 approximations!

- approx. E w/ this V
- $V \longmapsto V_{simple}(x)$

$\boxed{5}$ Goal: estimate g.s. energy E_0.

$$\underset{\text{(energy)}}{H} = \frac{p^2}{2m} + V(x)$$



classical ground state has $H = V_0$. $[p=0,\ x=x_0]$.

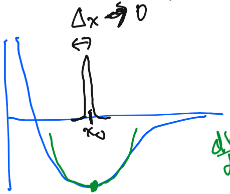
Heisenberg uncertainty: in QM

$$\Delta x\, \Delta p \geq \frac{\hbar}{2}.$$

Evaluate: $\underbrace{H = \frac{\Delta p^2}{2m} + V(x_0 + \Delta x)}$?

6 If mass $m \to \infty$: $H = \frac{p^2}{2m} + V(x)$

Δp large, Δx smaller... $V \to V_0$.



Start w/ $V(x)$...

behavior near x_0...

expand in $\Delta x = x - x_0$... (Taylor)

$\frac{dV}{dx}$

$\downarrow$

$$V(x) = \underbrace{V(x_0)}_{V_0} + \underbrace{V'(x_0)}_{V'(x_0)=0}(x - x_0) + \underbrace{\tfrac{1}{2}V''(x_0)}(x - x_0)^2 + \dots$$

b/c minimum

$V''(x_0) = \frac{d^2V}{dx^2}\Big|_{x_0} > 0$.

$= m \cdot \omega^2$

$\omega = \sqrt{\frac{1}{m}V''(x_0)}$.

End: $V(x) \approx V_0 + \frac{1}{2}m\omega^2 (x - x_0)^2$

7 $H \to \underline{\frac{p^2}{2m} + V_0 + \frac{1}{2}m\omega^2(x-x_0)^2} \to \frac{\Delta p^2}{2m} + \frac{1}{2}m\omega^2\Delta x^2.$

Goal: minimize H constrained to $\Delta x \Delta p = \frac{\hbar}{2}$.

$\Delta p = \hbar/2\Delta x$

$$H \to \frac{\hbar^2}{8m}\cdot\frac{1}{\Delta x^2} + \frac{1}{2}m\omega^2\Delta x^2.$$

$$\frac{\partial H}{\partial \Delta x} = 0 = -\frac{\hbar^2}{4m}\frac{1}{\Delta x^3} + m\omega^2\Delta x, \quad \text{so} \quad \Delta x^4 = \frac{\hbar^2}{4m^2\omega^2}$$

$$\Delta x^2 = \frac{\hbar}{2m\omega}$$

Plug in: $H = \frac{1}{2}\left(\frac{1}{2}\hbar\omega\right) + \frac{1}{2}\left(\frac{1}{2}\hbar\omega\right) = \underbrace{\frac{1}{2}\hbar\omega.\ [+V_0]}_{\text{good approx if...}}$

$V \sim x^2$

(quantum) <u>harmonic</u> oscillator

(Casimir effect $\frac{\hbar\omega}{2}$ real)