

SPL 13

OVERVIEW

[LOC. 5.1]

- I) QUICK RE-DERIVATION OF $S = k \ln \Omega$
- II) RECIPE FOR QM PROBS.
- III) EXAMPLE: QUANTUM, FORCE-FREE PTCL IN AN α -POTENTIAL WELL
- IV) ALTERNATIVE DERIVATION OF OF PATHRIA'S

$$\Sigma(E, V, N) = \left(\frac{V}{h^3} \right)^N \left(\frac{2\pi m E}{(3N/2)!} \right)^{3N/2}$$

FOR N -INDEPENDENT QUANTUM PTCLS IN AN α -POTENTIAL WELL

I) RE-DERIVATION OF $S = k \ln \Omega$

a)

E_1	E_2
N_1	N_2
V_1	V_2

 $E^{(0)} = E_1 + E_2 = \text{fixed}$
 $N_1, N_2, V_1, V_2 \text{ fixed}$

b) $\Omega^{(0)} = \Omega^{(0)}(E_1 + E_2) = \Omega_1(E_1) \Omega_2(E_2)$

OR $\Omega^{(0)} = \Omega^{(0)}(E_1) = \Omega_1(E_1) \Omega_2(E^{(0)} - E_1)$

c) IS EQUIL $E^{(0)}$ $\Omega^{(0)}$ GOING TO A MAXIMUM

$$\therefore \frac{\partial \Omega^{(0)}}{\partial E_1} = \frac{\partial \Omega_1}{\partial E_1} \Omega_2 + \Omega_1 \frac{\partial \Omega_2}{\partial E_2} \frac{\partial E_2}{\partial E_1} = 0$$

d) $\therefore$ @ EQUIL

$$\frac{\partial \ln \Omega_1}{\partial E_1} = \frac{\partial \ln \Omega_2}{\partial E_2} = \beta$$

e) COMPUTE

$$TdS = dE + PdV - \sum_i \mu_i dN_i$$

and $d \ln \Omega = \frac{\partial (\ln \Omega)}{\partial E} dE + \frac{\partial (\ln \Omega)}{\partial V} dV + \sum_i \frac{\partial (\ln \Omega)}{\partial N_i} dN_i$ ($dE = dN_i = 0$)

st & sd apply to
same sys, & same de.

Loc 5.2

~~Complex~~

$$\frac{ds}{d(\ln \Omega)} = \frac{1}{T} \left[\frac{d}{d(\ln \Omega)} \right]^{-1}$$

$$= \frac{1}{BT}$$

$$\Rightarrow \left[\frac{ds}{d(\ln \Omega)} = \frac{1}{BT} \right] \text{ Assume } = K$$

II) Review of QM

1) Planck postulates

$$\begin{array}{l} \text{ptcl. wave prop.} \\ E = h\nu = \frac{h}{2\pi} 2\pi\nu = h\nu \\ p = \hbar k \end{array}$$

2) look for a wave funⁿ that $\psi(x,t)$
3) Discrete Relations - somehow captures particle-wave

Free ptcl example characteristics

$$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} = h\nu \quad \left[\begin{array}{l} \text{Discrete} \\ \text{ptcl.} \end{array} \right]$$

character
discrete
rel

$$\Rightarrow \frac{\hbar^2 \nabla^2}{2m} \psi = \hbar^2 \frac{k^2}{2m} \psi$$

$$\Rightarrow i\hbar \psi_{n,t} = \omega \hbar \psi_n \Rightarrow \left[-\frac{\hbar^2 \nabla^2}{2m} \psi \right] = i\hbar \psi_{n,t}$$

(Schrödinger)

5) Particle $\hat{p} = -i\hbar \nabla$

lec 5.3

6)

typical QM Recipe

a) Guess / formulate H for your system

$$H = \underset{\substack{\text{en.} \\ \text{for} \\ \text{sys}}}{KIN} + \underset{\substack{\text{en.} \\ \text{for} \\ \text{sys.}}}{Pot.}$$

b) Replace P 's in H

$$w/ \hat{P} = -i\hbar \nabla, \quad L's \quad w/ \quad \hat{L} = i\hbar \hat{L} \times \nabla$$

etc.) Finally, ~~for~~ ^{check} system Hamiltonian operators

~~if~~

$\hat{H}$

c) Solve Schrodinger's eqn:

$$\hat{H}\psi = i\hbar \psi_t$$

Important points

① Few analytical solns possible

② perturbation methods widely used

③ for stationary (= statistically stationary) problems

see 5.4

(ie problems in which
statistical props do not
 vary in time), assume

$$\psi = \tilde{\psi}(x) e^{-i\omega t}$$

(+) For stationary probs
 S.E. becomes:

$$\boxed{\hat{H} \tilde{\psi}(x) = \hbar \omega \tilde{\psi}(x)} \quad (4.0)$$

or from PEdB postulate,

$$\boxed{E = \hbar \omega}$$

$$\boxed{\hat{H} \tilde{\psi}(x) = E \cdot \tilde{\psi}(x)} \quad (4.1)$$

(+) EQ (4.1) (or 4.0) ~~is~~ represents
 an eigenvalue / eigen fn
problem

i) TO ANY given set of
QUANTUM NUMBERS, $\{l, m, n, p, q, \dots\}$
 arising in a given
 problem, there
 corresponds an

lec 5.5

Eigenvalue, $E = E_{l,m,p,q,\dots}$

Discrete set of ~~arises~~ ~~dis~~ arises
 $\{E_{l,m,n,p,q,\dots}\}$

due to Boundary conditions
 imposed on $\tilde{\psi}(x)$. More

later.

~~IV~~ (IV) DERIVATION OF PATTERIA EQ 1.4.5

In order to follow

Patricia in his examination
 of an ideal gas -

Sec. 1.4 - we must first
 recover his formula for
 the energy eigenstates
 for a single force-free
 ptcl. in a box:

$$\begin{aligned} \boxed{1.4.5} \quad E &= E(n_x, n_y, n_z) = \frac{h^2}{8mL^2} \Omega_{n_x, n_y, n_z} \\ &= \frac{h^2}{8mL^2} [n_x^2 + n_y^2 + n_z^2] \\ n_x, n_y, n_z &= 1, 2, 3, \dots \end{aligned}$$

lec 5.6

1st postulate Hamiltonian:

- a) 1 for 1 free ptcl. in an infinite potential well,

$$H = \frac{\hat{P} \cdot \hat{P}}{2m}$$

$$V(x,t) = \begin{cases} 0 & \text{in Box} \\ \infty & \text{outside Box} \end{cases}$$

b) $\hat{H}\psi = i\hbar\psi_{,t}$

$$\frac{\hat{P} \cdot \hat{P}}{2m} \psi(x,t) = i\hbar\psi_{,t}$$

$$\hat{P} \equiv -i\hbar\nabla$$

$$\Rightarrow \left[-\frac{\hbar^2}{2m} \nabla^2 \psi = i\hbar\psi_{,t} \right] \quad (6.1)$$

- c) Assuming that the probability of observing the ptcl

@ the box boundaries

is 0, $(P(\text{walls}, t) = \psi^*(x,t) \psi(x,t))$

then we get B.C.'s on ψ :

B.C. 1,2

$$\psi(x=0, y, z, t) = \psi(L_x, y, z, t) = 0$$

B.C. 3,4

$$\psi(y=0, x, z, t) = \psi(L_y, x, z, t) = 0$$

B.C. 5,6

$$\psi(x, y, 0, t) = \psi(x, y, L_z, t) = 0$$

(6.2)

lec 5.7

d) Focus on the case where statistical properties of the ptcl. are stationary in time.

Thus, look for a soln for $\psi(x, t)$ of the form.

$$\boxed{\psi(x, t) = \tilde{\psi}(x) e^{-iEt/\hbar}} \quad (7.1)$$

~~e) plug 7.1 into (6.1)~~

e) ~~From (6.1)~~ then

$$\boxed{-\frac{\hbar^2}{2m} \nabla^2 \tilde{\psi}(x) = E \tilde{\psi}(x)} \quad (7.2)$$

E from PE def

f) By inspection, ^(of B.C.'s in 6.2) or sepn of variables, or trial and error, assume

$$\boxed{\tilde{\psi}(x) = A \sin(k_x x) \sin(k_y y) \sin(k_z z)} \quad (7.3)$$

Lec. 5.8

⊕ plug (7.3) into (7.2) to get:
the dispersion relation:

$$\left[\frac{\hbar^2}{2m} (k_x^2 + k_y^2 + k_z^2) \tilde{\psi}(x) = E \tilde{\psi}(x) \right] \quad (8.1)$$

cancel cancel

⊕ in order to satisfy the
B.C.'s in (6.2)

$$\begin{aligned} (8.2) \quad & \cancel{K_x L} \quad K_x L = n_x \pi & n_x &= 0, 1, 2, 3 \\ & K_y L = n_y \pi & n_y &= " \\ & K_z L = n_z \pi & n_z &= " \end{aligned}$$

⊕ ∴ from (8.1) & (8.2):

$$\frac{\hbar^2 (2\pi)^2 (\pi)^2}{2mL^2} [n_x^2 + n_y^2 + n_z^2] = E$$

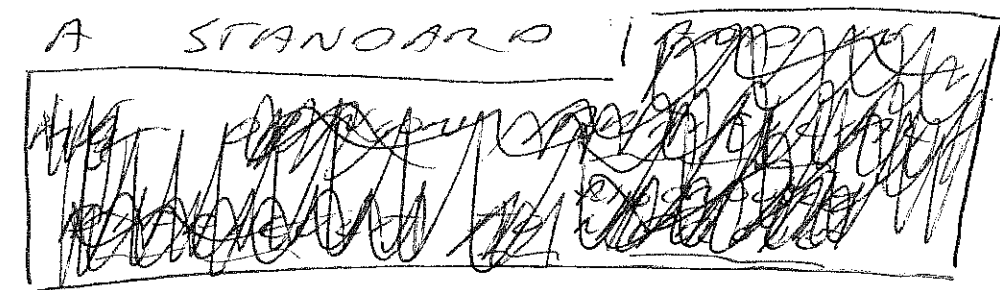
$$\Rightarrow \left[\frac{\hbar^2}{8mL^2} [n_x^2 + n_y^2 + n_z^2] = E = E(n_x, n_y, n_z) \right]$$

LEC. 5.9

IV) ALTERNATE DERIVATION
OF PATHRIA'S 1.4.17:

$$\Sigma(N, V, E) \approx \left(\frac{V}{h^3}\right)^N \frac{(2\pi m E)^{3N/2}}{(3N/2)!}$$

A) PATHRIA USES (I'M GUESSING)



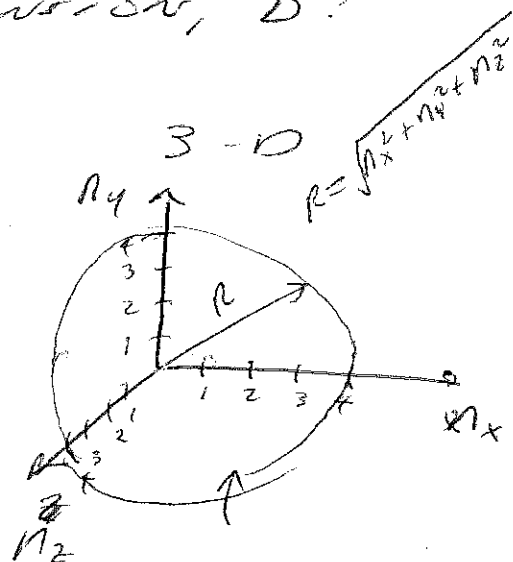
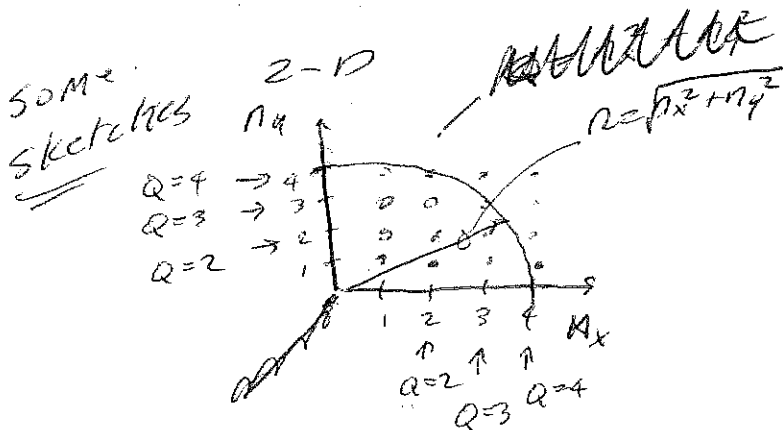
APPROACH FOR GETTING
1.4.17, i.e., THE GEOMETRICAL
APPROACH IN APPENDIX C.

B) MY APPROACH LEADS TO
AN EXPN THAT'S DIFFERS
FROM PATHRIA IN ONE
CRUCIAL TERM, A $\left(\frac{1}{N}\right)^{3N/2}$.
THIS DIFFERENCE, IN TURN,

[L52. 5.10]

LEADS TO A PHYSICALLY INTERESTING
INSIGHT (AND FIX FOR THE
DISCREPANCY).

- 1) ~~NOT~~ PROCEED BY
INDUCTION; FIRST ~~DE~~ FIGURE
OUT THE NUMBER OF
LATTICE POINTS IN THE
POSITIVE QUADRANT OF
~~THE~~ IN ~~VARIOUS~~ SPACES OF
VARIOUS DIMENSION, D :



(a) $Q = \text{NO OF TIC} = R = \sqrt{n_x^2 + n_y^2 + n_z^2}$
MARKS ON
EACH AXIS

FOR $N=1$
3-D

(b) LET $E^* \equiv n_x^{(1)2} + n_y^{(1)2} + n_z^{(1)2} + \dots$
 $+ n_x^{(N)2} + n_y^{(N)2} + n_z^{(N)2}$

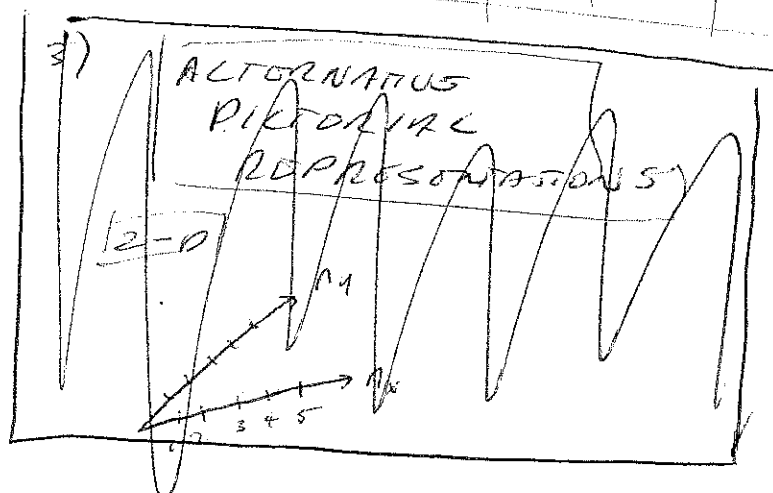
LET $E^* \equiv \frac{8\pi L^2 E}{h^2}$ $\therefore E \text{ GIVEN} \Rightarrow E^* \text{ GIVEN}$

2)

TABLE SHOWING NO. OF QUANTUM STATES SATISFYING $E(n_x^{(1)}, n_y^{(1)}, n_z^{(1)}, \dots, n_x^{(N)}, n_y^{(N)}, n_z^{(N)}) \leq E^*$					
DIMENSION	NO. OF AXIS TILLS				
	(2)	(3)	(4)	...	(Q)
2-D	4	9	16	...	Q^2
3-D	8	27	64	...	Q^3
M-D	2^M	3^M	4^M	...	Q^M
$M=3N$	2^{3N}	3^{3N}	4^{3N}	...	Q^{3N}

Lec 5.10

$\tilde{E}^* \leq E^*$



3) FROM THE FIGURES ON PG 10 AND THE TABLE ABOVE, WE CONCLUDE ~~THE~~ THE FOLLOWING:

- a) $R = Q$ (11.1) QUANTUM FOR N-IND. PTLS
- b) NO. OF STATES SATISFYING
- (11.2) $\tilde{E}^* = \sum_{i=1}^{3N} n_i^2 \leq E^* = \frac{8\pi^2 E}{h^2}$ IS
- Q^{3N}

Cor. 5.12

c) SO BY LETTING THE
NUMBER OF QUANTUM
STATES ASSOCIATED WITH
N independent p.t.s
IN A BOX BE $\Sigma = \Sigma(N, V, E)$
WE CAN FIND:

$$\Sigma(N, V, E) \approx Q^{3N} \quad (2.1)$$

d) ~~THE~~ $R = Q$ ^{from (2.1)} has a clear
geometric interpretation in
2-D and 3-D - see P. 55
on pg. 5.10. IN HIGHER

dimensions, we can still
~~interpret~~ Q as a radius,
interpret Q as a radius,

R -- when all n_i 's except
1 ^(say n_1) are equal 0, then we
have:

$$(2.2) \quad R = n_1 \quad (\text{geometric view})$$

BUT we also have from b)
on pg 5.10

Lec 5.13

$$E^* = \epsilon_I^2 = \frac{8ML^2E}{h^2} \quad (13.1)$$

SO, COMBINING $I=1,2,3,\dots$ or $3N$ (12.2) & (13.1),
we get

$$R^2 = \frac{8ML^2E}{h^2} \quad (13.2)$$

⊕ FINALLY, COMBINING, ~~(11.1)~~
~~AND~~ (13.2) WE GET!

$$\underbrace{Q}_{(11.1)} = \underbrace{R}_{(13.2)} = \sqrt{\frac{8ML^2E}{h^2}} \quad (13.3)$$

SO THAT (12.1) BECOMES:

$$(13.4) \quad \underbrace{\sum (N, V, E)}_{(12.1)} \approx \underbrace{Q^{3N}}_{(13.3)} = \left(\frac{8ML^2E}{h^2} \right)^{\frac{3N}{2}}$$

OR *

$$\sum (N, V, E) \approx \left(\frac{V}{h^3} \right)^N (8ME)^{3N/2} \quad (13.5)$$

* $V = L^3$

⊕ INTERPRETATION IN LEC 6