LECTURE 14/36 OCT-7-02

DE BROGLIE

HEINSENBERG UNCERTAINTY

POSTULATES IN Q. M

PARTICLE IN A BOX

BACKGROUND: OXTOBY CH 15

READ: NEXT LEC: GRAY, CH 1, p21-38

DE BROGLIE

PARTICLES OR WAVES?

	PARTICLE-LIKE	WAVE-LIKE
MATTER PARTICLES	p	?
WAVES E&M	PHOTONS $p = \frac{h}{\lambda}$	λ

FOR A PARTICLE WITH MOMENTUM p, WE ASSOCIATE A WAVELENGTH

$$\lambda = \frac{h}{p}$$

Heisenberg Uncertainty (Indeterminancy) Principle

One cannot measure the position x and the momentum in the x direction with infinite accuracy [$\Delta x = 0$ and/or $\Delta p_x = 0$] at the same time.

If we are able to increase the accuracy in position [$\Delta x \to 0$], the accuracy in momentum will decrease [$\Delta p_x \to \infty$] in such a way that

$$\Delta x \, \Delta p_x \geq \frac{h}{4\pi}$$

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QUANTUM MECHANICS: WHEN IS IT REALLY NECESSARY?

There was a time when the newspapers said that only twelve men understood the theory of relativity. I do not believe there was ever such a time. There might have been a time when only one man did, because he was the only guy who caught on, before he wrote his paper. But after people read the paper, a lot of people understood the theory of relativity in some way or other, certainly more than twelve. . . . On the other hand, I think I can safely say that nobody understands quantum mechanics. – *Richard Feynman*

ı Section 4, we found that many spectral properties ordinarily introduced y quantum mechanics could be understood in terms of simple classical ıodels based on a weight on a spring. The classical model fails, however, ı a number of areas important to biophysical applications (and in other reas of interest to different audiences, such as physicists). For example, classical electron on a spring oscillates at only *one* natural frequency, 'hile the actual electron on a spring in a simple hydrogen atom vibrates t an *infinite* number of "natural" frequencies – quantum mechanics proides the means for predicting the number and magnitudes of those freuencies (Chapter 18). Once it is established that particles may possess nly certain, discrete (as opposed to continuous), "quantized" energies, ıere immediately arises the statistical problem of deciding how many articles possess each particular energy, given that the total number of articles and the total energy of the collection of particles is constant. The esulting Boltzmann distribution (Chapter 19) then predicts a variety of ıolecular properties such as average electric dipole moment that are unbt..ıable from classical mechanics, and lead in a natural way to the undertanding of lasers and other nonequilibrium situations. Finally, the effect f applied or naturally existing fluctuating electric or magnetic fields on ransitions between energy levels (related to spectral absorption intensities ınd associated chromophore and "reporter group" experiments) follow from

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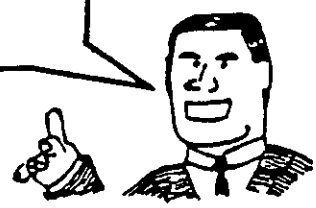
The One-Electron Atom

Apparently there is colour, apparently sweetness, apparently bitterness; actually there are only atoms and the void.

Democritus, 420 B.C.

6/14

"In just 38 months, you can earn big PROFIT$ as a fully trained QUANTUM MECHANIC!"



Learn secrets of QUANTUM MECHANICS in your own home, in your spare time, without quitting your present job!

DO YOU HAVE WHAT IT TAKES TO BE A QUANTUM MECHANIC?

Not just anyone can be a quantum mechanic. It takes determination, drive, imagination and money. Most of all, money. Bob is putting a son through medical school.

NATION CRYING FOR FULLY TRAINED QUANTUM MECHANICS

That's right, friend, the nation is crying for fully trained quantum mechanics. Can you hear it? You can't? Well be very still. Listen, off in the distance. "Wahhh!" Hear that? That's the nation crying for quantum mechanics.

QUANTUM MECHANICS EAT STEAK

Yep, quantum mechanics make big bucks. Heavy bread. They're rolling in dough. They carry big wads of 10's and 20's in their pockets. A lot of MONEY. They drive Cadillacs and buy their wives minks. And they eat steak.

THIS COURSE TEACHES YOU ALL YOU NEED TO KNOW, EVERYTHING. THERE ISN'T A SINGLE THING ABOUT QUANTUM MECHANICS LEFT OUT.

Wrong, electron breath! But it's close. We teach you a whole bunch of stuff. Mesatron balancing. Quark reallignment. Neutrino lubrication. Proton tune-up. How to use a molecule wrench.

YOU GET PROFESSIONAL EQUIPMENT TO LEARN WITH

You will receive a professional cyclotron, actual atoms, a years' supply of Preparation A for your atomic piles, back issues of Scientific American to July, 1957 and a bill for your mailman's hernia operation. Not to mention our bill for $675. Which is cheap when you consider how proud you'll be to hear your son say, "My daddy's a Quantum Mechanic!"

—GUARANTEE—

I hereby guarantee that, without a doubt, this is the only course of its kind in the world. You'll be completely satisfied, or I'll cheerfully keep your money.

Bob

LISTEN TO WHAT THESE SATISFIED CUSTOMERS SAY!

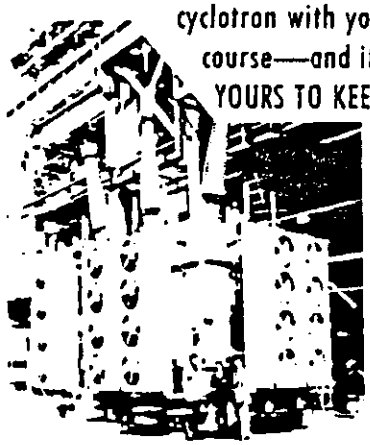
"Like, you know, this course, you know, it like, uh, expanded my consciousness, you know. And I need all the consciousness I can get, you know?"
PAT HEAD, San Francisco, Cal.

"One of my most proud moments was getting my diploma last May. I enrolled right after the war. That was the Big One, son. W.W. II!"
"POP" CHERRY, Sun City, Ariz.

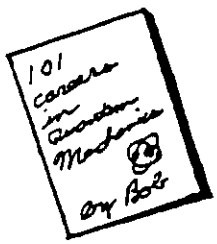
"I used to be Prime Minister of a major European nation. Then I took this course. Now I drive a big car, eat steak, and make over $6.00 an hour!"
HARRY DEAN II, Tater, Ark.

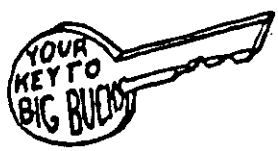
NO RISK!

You get this Professional cyclotron with your course—and it's YOURS TO KEEP!



Send NOW for this FREE BROCHURE!





NO OBLIGATION - NO SALESMAN WILL CALL

BOB'S SCHOOL OF QUANTUM MECHANICS

BOB'S SCHOOL

A DIVISION OF BOB'S CONOCO SERVICE STATION
7036 STATE ROAD 29
EAST BELCH, NORTH DAKOTA 51106
•Approved by Peruvian Ministry of Agriculture
•Approved by Bob

MAIL COUPON NOW
Bob's School of Quantum Mechanics
7036 State Road 29
East Belch, ND 51106

Dear Bob,

Enclosed please find my $16.95 in cash (no check or money order, please). PLEASE RUSH me my FREE BROCHURE on an exciting carreer in QUANTUM MECHANICS. I understand if I am not completely satisfied, I have been had.

Name_____
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APPROVED FOR VETERANS
of the Spanish-American War

Reprinted from *Purdue Engineer Magazine*

QUANTUM MECHANICS

MECHANICS OF PARTICLES BEHAVING LIKE WAVES

WHAT IS THE WAVE EQ. FOR PARTICLES?

POSTULATE I

SCHRODINGER EQ.

$$\hat{H}\Psi = E\Psi$$

Ψ IS A MATHEMATICAL FUNCTION THAT REPRESENTS A PARTICLE'S BEHAVIOR LIKE A WAVE

$\hat{H} \equiv$ HAMILTONIAN

$\hat{H} = \hat{K} + \hat{V}$

$\hat{K} =$ KINETIC ENERGY $= \dfrac{\hat{p}^2}{2m}$

$\hat{V} =$ POTENTIAL ENERGY

$\hat{p} \equiv ?$

$\hat{p}_x = -i\hbar \dfrac{d}{dx}$

$\hbar = \dfrac{h}{2\pi}$

IN 3-d $\quad \hat{p}^2 = -\hbar^2 \nabla^2$

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

E = ENERGY LEVELS

POSTULATE II

$$\text{PROB} \equiv |\psi|^2 dV = |\psi(\underset{\sim}{r})|^2 dV$$

PROBABILITY OF FINDING THE ELECTRON WITHIN A VOLUME dV AROUND $\underset{\sim}{r}$

COROLLARY

$$\int_{\text{VOL}} |\psi|^2 dV = 1$$

POSTULATE III

THE AVERAGE OF ANY OBSERVABLE $\hat{\Theta}$ IS GIVEN BY

$$\int_{VOL} \psi^* (\hat{\Theta}\psi)\, dV \equiv \langle \hat{\Theta} \rangle$$

WHERE ψ^* IS THE COMPLEX CONJUGATE OF ψ ($i \equiv \sqrt{-1} \longrightarrow -i$)

EXAMPLE

$$\hat{p}_x = -i\hbar \frac{d}{dx}$$

$$\hat{p}_x^2 = -\hbar^2 \frac{d^2}{dx^2}$$

$$\langle \hat{p}_x^2 \rangle = \int_{VOL} \psi^*(x) \left[-\frac{\hbar^2 d^2}{dx^2} \psi \right] dx$$

Particle in a Box

(classical analogy → vibrating string).

Biological applications

a) Behavior of π electrons that are delocalized over large portions of a molecule.

i) Linear polyenes (carotenoids, retinal).
ii) Planar porphyrins (heme, chlorophyll).
iii) Large Aromatic Hydrocarbons.

b) Conduction electrons that may move over extensive regions of a biopolymer.

c) Exchange of protons involved in hydrogen bonding between two nucleophilic atoms as between the oxygen of adjacent water molecules.

PARTICLE IN A BOX

MODEL OF DELOCALIZED π electrons IN LINEAR CONJUGATED HYDROCARBONS

BUTADIENE

$$H_2C=CH-CH=CH_2$$

C=C 135 pm pm = 10^{-12} m

C–C 154 pm

CARBON RADIUS 77 pm

$$L = 578 \text{ pm}$$

EXPERIMENT: ABSORPTION $\bar{\nu} = 4.61 \times 10^4 \text{ cm}^{-1}$

π-e IN BUTADIENE ARE FREE.

$V(x) = 0$