Select/Special Topics in Atomic Physics
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Introductory Lecture about this Course

Greetings, a very happy welcome to this course on Special Topics in Atomic Physics or preferred to call it as Select Topics in Atomic Physics, because the subject is vast and there is only a certain selection of topics that one could do in a course.

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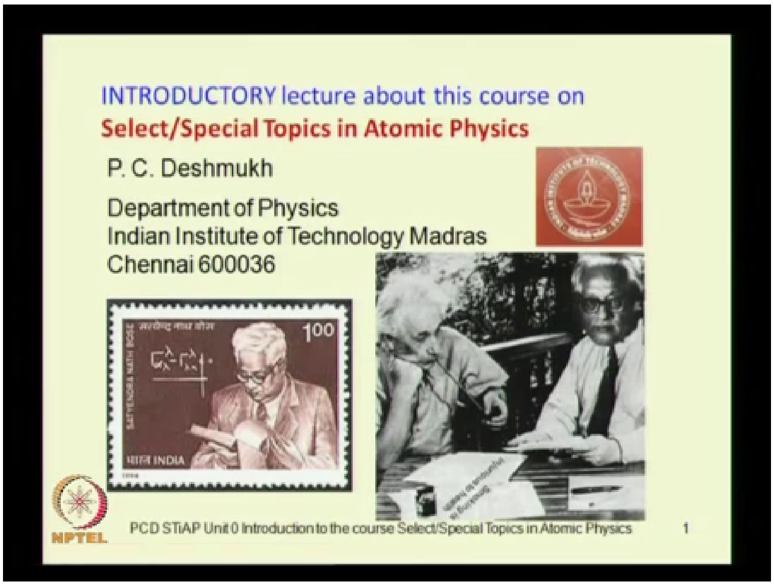

INTRODUCTORY lecture about this course on

Select/Special Topics in Atomic Physics

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And we begin with a tribute to Satyendranath boss, and of course to Albert Einstein, who has perhaps more than anybody else contributed to the both of quantum mechanics in the last century.

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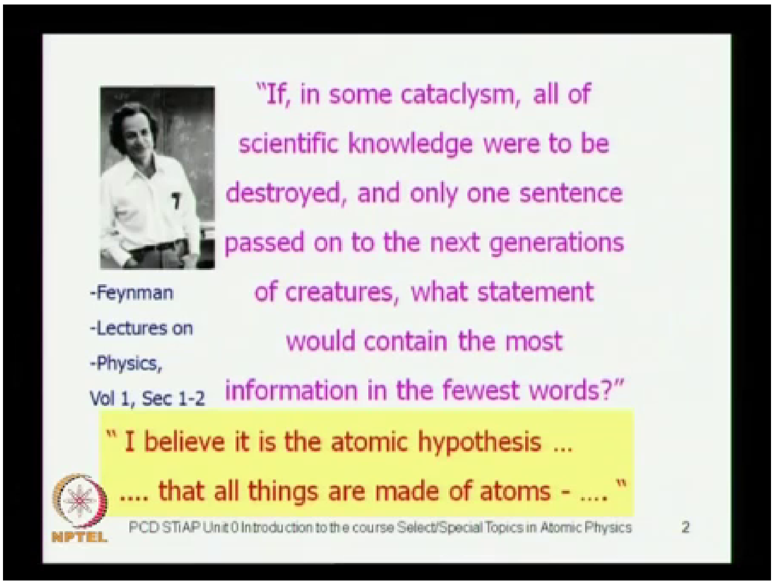

"If, in some cataclysm, all of scientific knowledge were to be destroyed, and only one sentence passed on to the next generations of creatures, what statement would contain the most information in the fewest words?"

-Feynman
-Lectures on
-Physics,
Vol 1, Sec 1-2

" I believe it is the atomic hypothesis ...
.... that all things are made of atoms - .... "

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And I begin with the course from Feynman, he asks the question that, if in some cataclysm, all of scientific knowledge were to be destroyed and only one sentence passed on to the next generation of creatures. What statement would contain the most information in the fewest words, Feynman goes on to answer this question and he says that, it is atomic hypothesis, that all things are made of atoms and this is what you will find in volume one of Feynman lectures.

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Dalton.... Mendeleyev ...
Angstrom ... Balmer .. Rydberg ..
Einstein .. Heisenberg.. Schrodinger.... Bohr
.. Pauli .. Born .. ..
Som
Hartree .. Fock ..Dirac ...
Chandrasekhar
Fano ... Seaton... Dalgarno ...
Bose...Cornell-Wieman ..Ketterle.. Webb..

Special Lecture

NPTEL / NKN

http://www.youtube.com/watch?v=2sP5C7Eh8HY

An Odyssey in Atomic Physics

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So, quite obviously, atomic physics is a very exciting field and the subject grow along with quantum mechanics in the last century. Large number of scientist, here is an experimentalist have contributed to growth of this field. And I have reviewed some of the excitement in the development in atomic physics in a talk, which was given as a special lecture for the NPTEL and the national knowledge network. This is available of the, you tube called an Odyssey in atomic physics.

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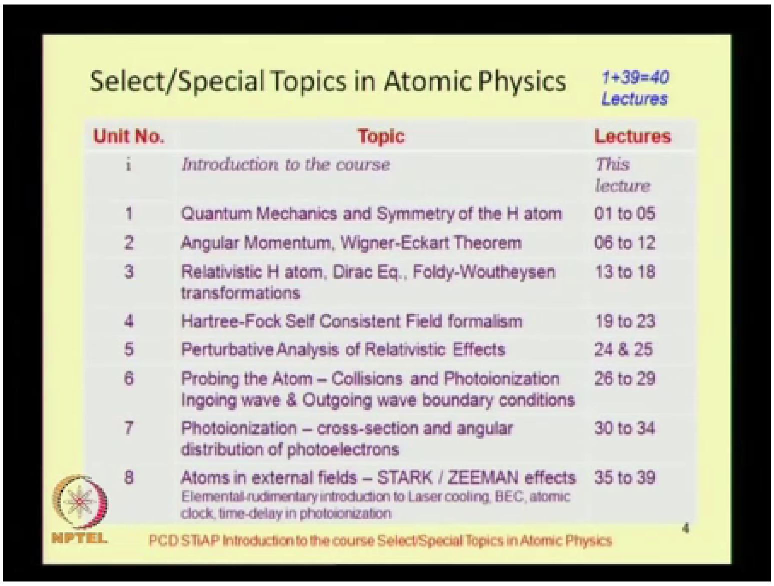

Select/Special Topics in Atomic Physics

1+39=40 Lectures

Unit No.	Topic	Lectures
i	*Introduction to the course*	*This lecture*
1	Quantum Mechanics and Symmetry of the H atom	01 to 05
2	Angular Momentum, Wigner-Eckart Theorem	06 to 12
3	Relativistic H atom, Dirac Eq., Foldy-Woutheysen transformations	13 to 18
4	Hartree-Fock Self Consistent Field formalism	19 to 23
5	Perturbative Analysis of Relativistic Effects	24 & 25
6	Probing the Atom – Collisions and Photoionization Ingoing wave & Outgoing wave boundary conditions	26 to 29
7	Photoionization – cross-section and angular distribution of photoelectrons	30 to 34
8	Atoms in external fields – STARK / ZEEMAN effects Elemental-rudimentary introduction to Laser cooling, BEC, atomic clock, time-delay in photoionization	35 to 39

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4

But, what we will do in this course is to go through some of the important areas, on which studies in atomic physics are based and this course will be covered in 40 lectures. So, in addition to today, today is introductory lecture, there will be 39 lectures that will follow and we will cover this in 8 units. In the 1st unit, I will discuss the quantum mechanics and symmetry of the hydrogen atom. In the 2nd unit, I will discuss angular momentum algebra and quantum mechanics of angular momentum in Wigner Eckart theory.

In the 3 rd unit, we will study the relativistic hydrogen atom, the Dirac equation and the Foldy Woutheysen transformations. In the 4th unit, we will go over to many electron atoms and talk about the self consistence field and the Hartree Fock method of getting many electron wave functions. In unit 5, we will talk about perturbative analysis of relativistic effects and in unit 6, we will study how an atom is probed and one could use, either collisions or photo ionization to study this.

And in unit 7, we will discuss photo ionization in some further details, in which we will use the boundary conditions, which we would develop in unit 6, because for photo ionization, you need one set of boundary conditions opposed to another set of boundary conditions for collision. And then finally, in unit 8, we will study about atoms in external fields, we will talk about the STARK effect or ZEEMAN effect. And also provide a very rudimentary in introduction to some exciting phenomenon like laser cooling, the Bose-Einstein condensation and the atomic clocks, attosecond metrology and so on.

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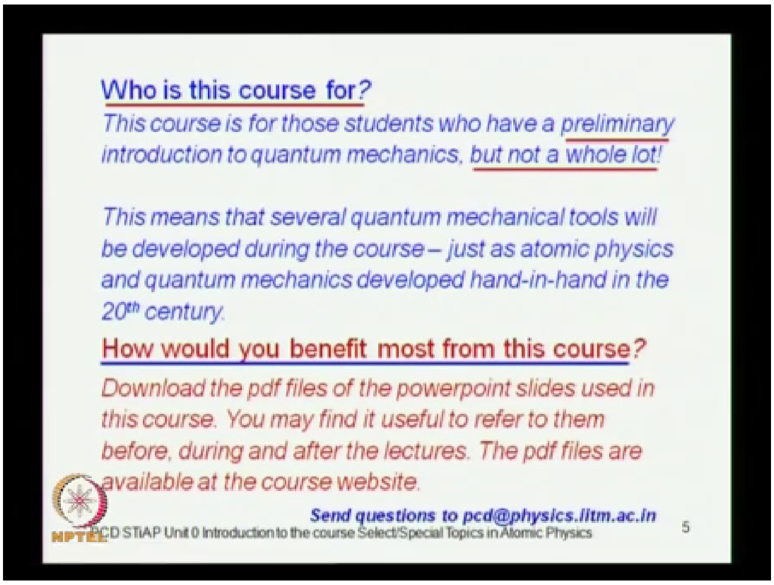

Who is this course for?

This course is for those students who have a preliminary introduction to quantum mechanics, but not a whole lot!

This means that several quantum mechanical tools will be developed during the course – just as atomic physics and quantum mechanics developed hand-in-hand in the 20th century.

How would you benefit most from this course?

Download the pdf files of the powerpoint slides used in this course. You may find it useful to refer to them before, during and after the lectures. The pdf files are available at the course website.

NPTEL

Send questions to pcd@physics.iitm.ac.in

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So, I will give a very brief overview of, what we are going to do in this course and how we will do it. But, first of all let me explain, who these courses meant for and I will like to inform or suggest that, this course is best suited for those, who have got some introduction to quantum mechanics, but not whole lot. Because, the subject of quantum mechanics and atomic physics develop together in the last century and a foundation for a course in atomic physics requires a strong background in quantum mechanics.

So, some of it will be developed as an integral part of the course, so you do need a little bit of introduction to quantum mechanics, but perhaps not a whole lot, if you already know a lot, you perhaps no need this course at all. Then, I will also like to mention, how to benefit more from this course, because I am going to be using the course material is developed and I will be using some of these PowerPoint slides for this course and these will be uploaded as PDF files on the course webpage.

So, it is a good idea to refer to this PDF files, you do not have to sit down and take notes during the class, but it is a good idea to refer to these PDF files before the lectures, during the lectures, after the lectures. And in the class, just concentrate on discussion, ask questions, have conversation, that is the best way to take this course. Now, of course if you have any question at any point, you should send them to me.

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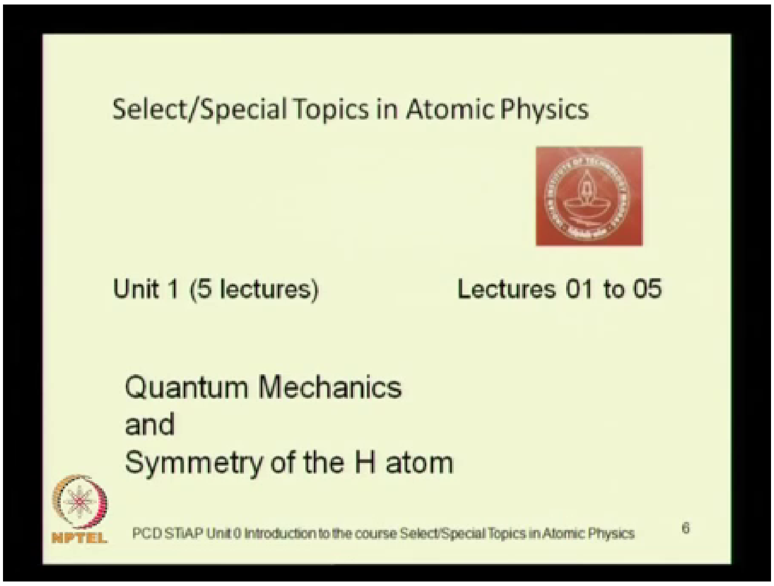

Select/Special Topics in Atomic Physics

Unit 1 (5 lectures)

Lectures 01 to 05

Quantum Mechanics
and
Symmetry of the H atom

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6

And I will now give an brief overview, what you will do unit 1, which will be on the quantum mechanics and symmetry of the hydrogen atoms.

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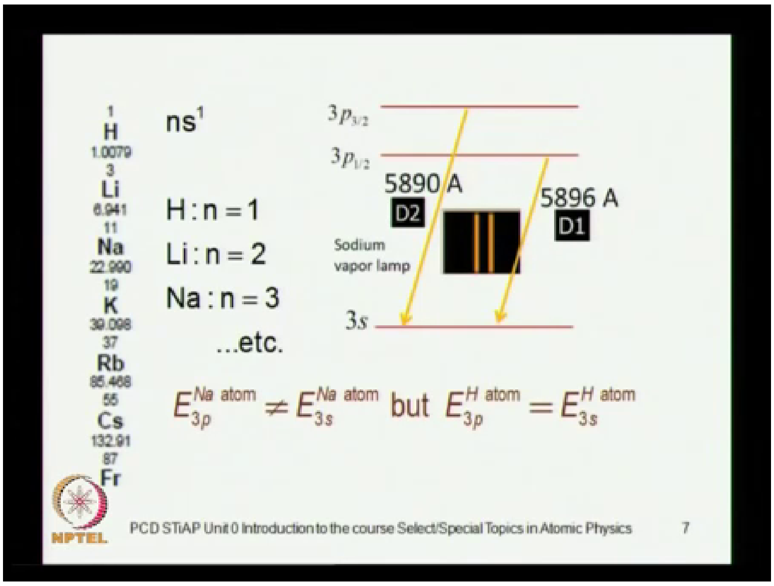

ns^1

H : n = 1

Li : n = 2

Na : n = 3

...etc.

$E_{3p}^{Na\ atom} \neq E_{3s}^{Na\ atom}$ but $E_{3p}^{H\ atom} = E_{3s}^{H\ atom}$

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7

So, the hydrogen atom along with alkali metal atoms belongs to the first group and they all have an outer n s 1 electronic configuration. All the alkali atoms like sodium atom, rubidium atom, cesium atom, you know these are all, they have all the similar structure and one of the thing, which is used, which is very well known about the speck of these atoms are the famous D 1 D 2 lines of the alkali atoms. Sodium atom, rubidium atom, cesium atom, all of them have got the D 1 D 2 lines, hydrogen does not, although it belongs to the same group.

And the question is, where have D 1 and D 2 lines of hydrogen disappear and the reason of course is that, the 3 p and 3 s energy levels of the hydrogen atoms are degenerate. Whereas, for other alkali atoms, the outer n p and outer n s, where n s 3 for sodium, but it is 2 for lithium and then, so on. So, for rubidium, cesium and so on, so the outer n p and n s levels are not degenerate and you do need a difference in the energies of n p and n s to have d to p transition.

There is further spin orbit spreading, but that is the matter of detail, which we will also be discussing it in separate unit, which is relativistic effect. But, essentially, one recognizes the fact that, the Eigen value spectrum of hydrogen is not just quantitatively, but qualitatively different from that of the other members of the group 1 atoms and this is the problem that, we will discuss in the first unit.

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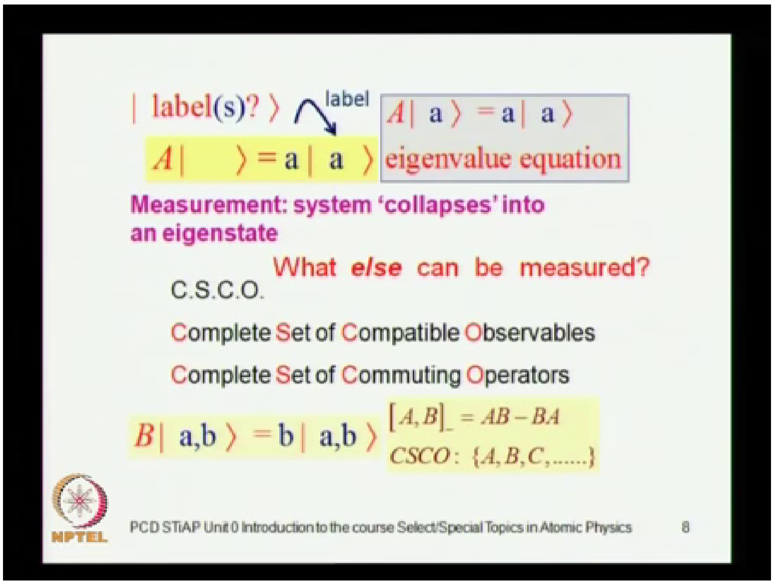

$| \text{label(s)?} \rangle$ $\curvearrowright$ label

$A| \quad \rangle = a|a\rangle$

$A|a\rangle = a|a\rangle$ eigenvalue equation

Measurement: system 'collapses' into an eigenstate

What *else* can be measured?

C.S.C.O.

Complete Set of Compatible Observables

Complete Set of Commuting Operators

$B|a,b\rangle = b|a,b\rangle$

$[A,B]_- = AB - BA$

$CSCO: \{A,B,C,......\}$

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We will introduce a complete set of commuting operators corresponding to complete set of compatible observations that can be made on the hydrogen atom, because this is what physicist looks for, to study any quantum systems. And we will therefore, introduce some basic foundation of quantum mechanics toward the beginning. So that, we know, what are the measurable properties of the hydrogen atom and how can we get a complete set of commuting operators.

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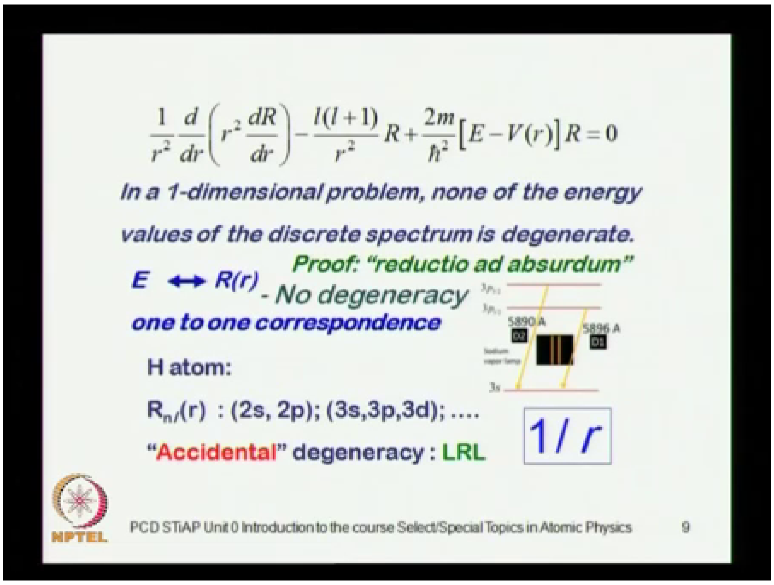

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)-\frac{l(l+1)}{r^2}R+\frac{2m}{\hbar^2}\left[E-V(r)\right]R=0$$

In a 1-dimensional problem, none of the energy values of the discrete spectrum is degenerate.

Proof: "reductio ad absurdum"

$E \leftrightarrow R(r)$ - No degeneracy

one to one correspondence

H atom:

$R_{nl}(r)$: (2s, 2p); (3s,3p,3d); ….

"Accidental" degeneracy : LRL

When we study this, it tells out that, if you look at the redial part of the Schrodinger equation for the hydrogen atom, it reduces to a one dimensional problem if you just look at the redial part. And then, by fundamental theorems in quantum mechanics, one know that, the energy spectrums is not degenerate, so there is a one to one correspondence between energy and wave functions for the hydrogen atom, according to this theorem. So, the degeneracy of the 2 s or 2 p levels in the hydrogen atom cannot be explained on the basis of this fundamental theorem. In fact, it is in contradiction to the consequence of this, the result of this theorem, so this is what, was called as accidental degeneracy.

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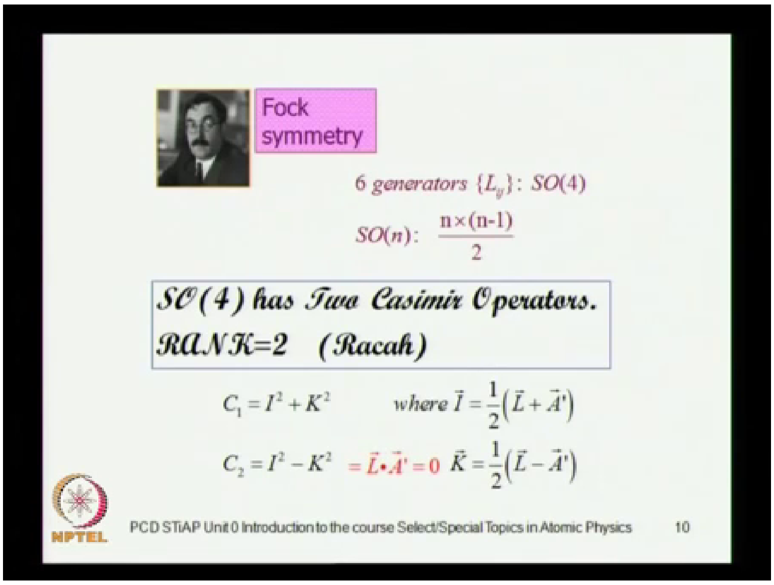

Fock symmetry

6 generators $\{L_{ij}\}$: $SO(4)$

$SO(n)$: $\frac{n\times(n-1)}{2}$

SO(4) has Two Casimir Operators.
RANK=2 (Racah)

$C_1 = I^2 + K^2$ where $\vec{I} = \frac{1}{2}(\vec{L} + \vec{A}')$

$C_2 = I^2 - K^2 = \vec{L}\bullet\vec{A}' = 0$ $\vec{K} = \frac{1}{2}(\vec{L} - \vec{A}')$

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But then, it is now understood in terms of this complete symmetry of the hydrogen atom, which is not just SO 3, but it is SO 4, this is sometimes called as a Fock symmetry. So, we will discuss the Fock symmetry of the hydrogen atom, we will develop the Casimir operators for this SO 4. And by studying the group properties of this particular symmetry, which is SO 4 symmetry of the hydrogen atom, we will get the Eigen value spectrum of the hydrogen atom. And we will recognize that, it explains the degeneracy in the hydrogen atom and it is not really an accidental degeneracy, there is a good physical reason for it.

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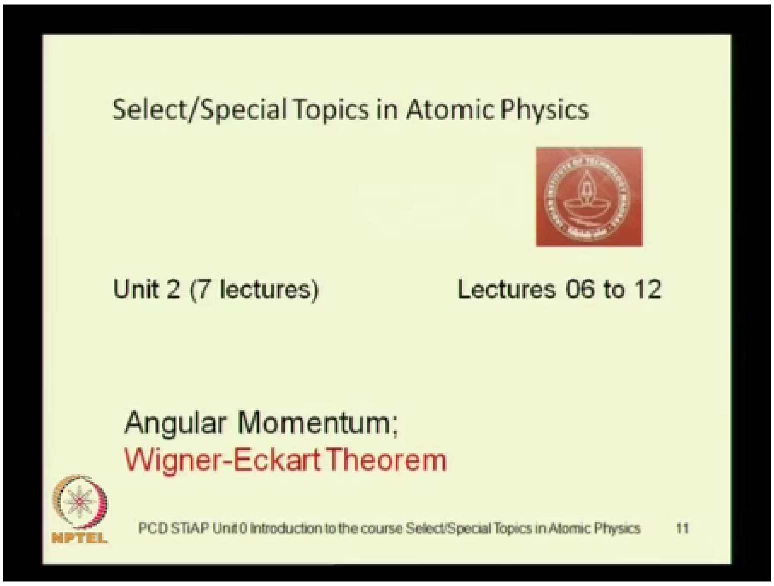

Select/Special Topics in Atomic Physics

Unit 2 (7 lectures) Lectures 06 to 12

Angular Momentum;
Wigner-Eckart Theorem

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Then, in unit 2, we will study angular momentum in quantum mechanics, angular momentum in classical mechanic is just r cross p. But, quantum mechanics requires different treatment of angular momentum and we will proceed to get a Wigner Eckart theorem as well.

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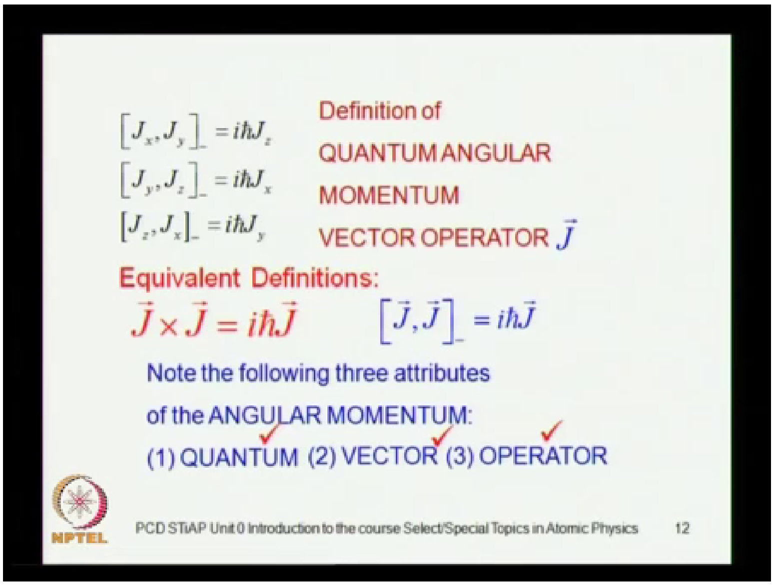

$[J_x, J_y]_- = i\hbar J_z$

$[J_y, J_z]_- = i\hbar J_x$

$[J_z, J_x]_- = i\hbar J_y$

Definition of
QUANTUM ANGULAR
MOMENTUM
VECTOR OPERATOR $\vec{J}$

Equivalent Definitions:

$\vec{J} \times \vec{J} = i\hbar \vec{J}$ $\qquad [\vec{J}, \vec{J}]_- = i\hbar \vec{J}$

Note the following three attributes of the ANGULAR MOMENTUM:

(1) QUANTUM (2) VECTOR (3) OPERATOR

So, we will give an appropriate definition of angular momentum in quantum mechanics and then, use this definition to deal with the algebra of angular momentum in quantum mechanics.

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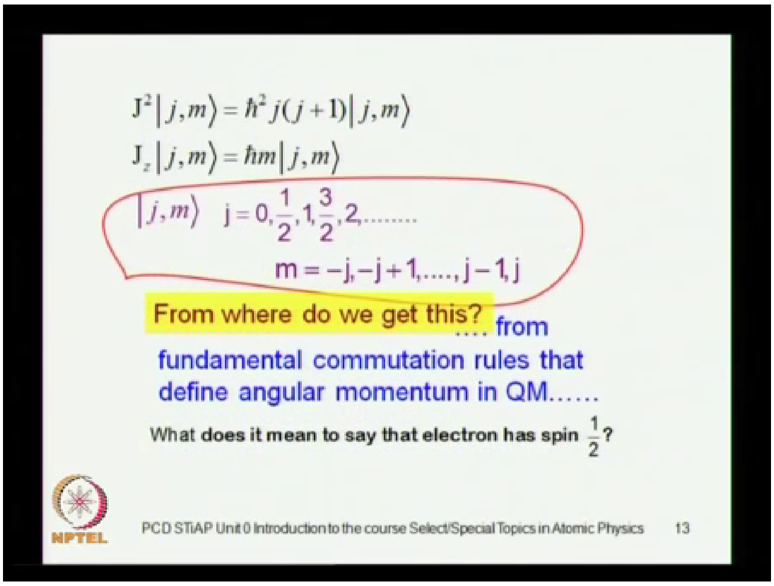

$J^2|j,m\rangle = \hbar^2 j(j+1)|j,m\rangle$

$J_z|j,m\rangle = \hbar m|j,m\rangle$

$|j,m\rangle \quad j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots\ldots$

$m = -j, -j+1, \ldots, j-1, j$

From where do we get this? .... from fundamental commutation rules that define angular momentum in QM......

What does it mean to say that electron has spin $\frac{1}{2}$?

So, we will discuss things like, what are the values of angular of momentum, now we all know from our earlier introduction in quantum mechanics show electron spin that, electron spin is 1 half. And one finds that, from the angular of momentum algebra, you can get this half integer quantum numbers like j equal to half, not only j equal to 0 1 2 3 etcetera, which are the integers, we can also get a half, 3 half and so on.

So, we will explain, how it is possible to get this half integer quantum numbers, we will also highlight the fact that, because this method accommodates half integer a quantum numbers. It is not the same as a sighing half integer quantum number to the electron, that has to come only from relativistic quantum mechanics, it comes from the Dirac equation, as we will discuss later in a different unit.

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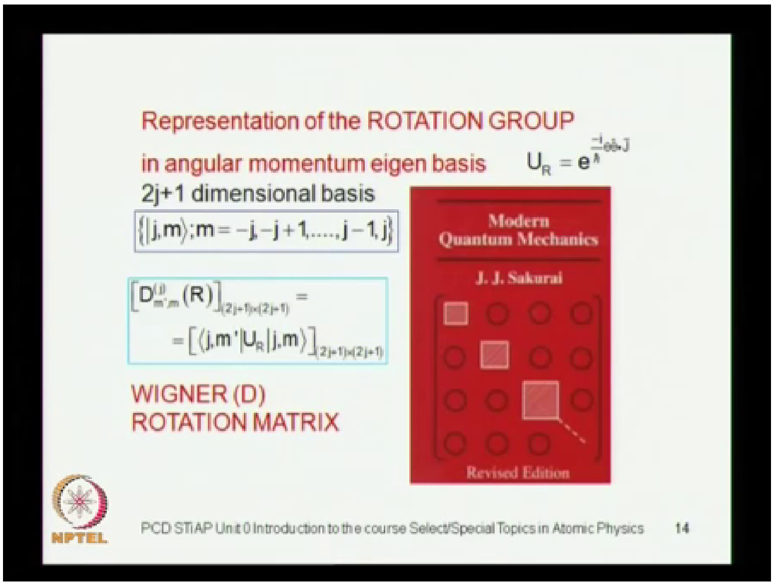

Representation of the ROTATION GROUP

in angular momentum eigen basis $U_R = e^{\frac{-i}{\hbar}\theta\hat{n}\cdot\mathbf{J}}$

2j+1 dimensional basis

$$\boxed{\{|j,m\rangle ; m = -j, -j+1, \ldots, j-1, j\}}$$

$$\left[D^{(j)}_{m',m}(R)\right]_{(2j+1)\times(2j+1)} = \\ = \left[\langle j,m'|U_R|j,m\rangle\right]_{(2j+1)\times(2j+1)}$$

WIGNER (D)
ROTATION MATRIX

Modern
Quantum Mechanics

J. J. Sakurai

Revised Edition

NPTEL

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So, we will have a fairly extensive discussion on the rotation group, because angular momentum is the generator of rotations. We will discuss the Wigner rotation matrices, which you find on the cover page of Sakurai's book. So, these are obviously important in quantum mechanics, in all aspects of mechanics, not just atomic physics, but in many other branches of quantum mechanics with applications in nucleus matrix and everywhere. So, these are the matrix elements of the rotation operator in angular momentum states and we will study properties of the Wigner rotation matrices element.

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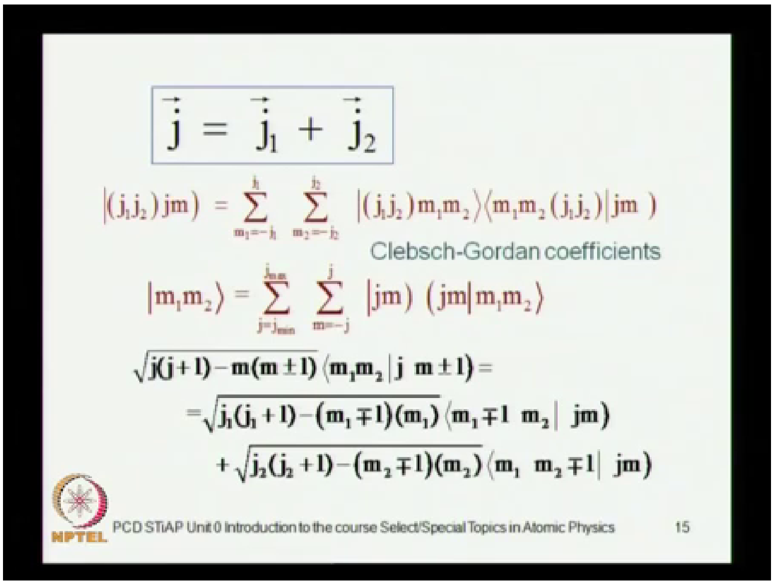

$$\boxed{\vec{j} = \vec{j}_1 + \vec{j}_2}$$

$$|(j_1j_2)jm) = \sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} |(j_1j_2)m_1m_2\rangle\langle m_1m_2(j_1j_2)|jm)$$

Clebsch-Gordan coefficients

$$|m_1m_2\rangle = \sum_{j=j_{min}}^{j_{max}} \sum_{m=-j}^{j} |jm)\ (jm|m_1m_2\rangle$$

$$\sqrt{j(j+1)-m(m\pm1)}\langle m_1m_2|j\ m\pm1) =$$
$$=\sqrt{j_1(j_1+1)-(m_1\mp1)(m_1)}\langle m_1\mp1\ m_2|\ jm)$$
$$+\sqrt{j_2(j_2+1)-(m_2\mp1)(m_2)}\langle m_1\ m_2\mp1|\ jm)$$

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We will then recognize that, the total angular momentum for any system is given by the quantum vector sum of all contributors to angular momentum. And you could have the orbital angular momentum as one contributor, you could have spin angular momentum as another contributor. In many particle system, you may have the orbital angular momentum and the spin angular of moment of all different particles and all of them would add up to give a net angular momentum of the quantum system.

And this is done by adding, now this is not just a vector addition, these are quantum vector operators, so one has to develop the tools to study this addition of these vector operators. And this is done using these coefficients called as the Clebsch Gordan coefficients, we will discuss how these Clebsch Gordan coefficients are obtained. You can get them from first principles, there are certain recursion relations, which are available, so that if you know the root coefficient, from this root coefficient, you can get the rest of the coefficients.

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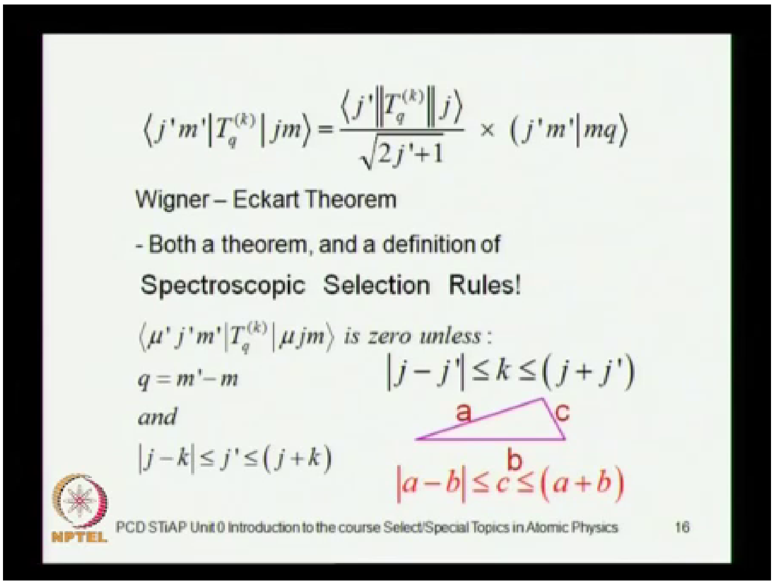

$$\langle j'm'|T_q^{(k)}|jm\rangle = \frac{\langle j'\|T_q^{(k)}\|j\rangle}{\sqrt{2j'+1}} \times (j'm'|mq)$$

Wigner – Eckart Theorem

- Both a theorem, and a definition of

Spectroscopic Selection Rules!

$\langle \mu' j'm'|T_q^{(k)}|\mu jm\rangle$ *is zero unless* :

$q = m' - m$

and

$|j-k| \le j' \le (j+k)$

$|j-j'| \le k \le (j+j')$

$|a-b| \le c \le (a+b)$

So, we will discuss some of these methods and then, we will establish the Wigner Eckart theorem and find that, it is extremely powerful tool in spectroscopy, because it tells us that, the probability amplitude for transition from a certain initial state to final state, which is what we investigate in spectroscopy. This probability amplitude can be factored into two pieces, a physical part which is called reduced matrix elements and a geometrical part, which is contained in the Clebsch Gordan coefficient.

So, this in fact, goes on to give us selection rules, the spectroscopic selection rules, like the dipole selection rules are the selection rules for the quadruple transition and so on. So, all kinds of different selection rules come out from the application of Wigner Eckart theorem.

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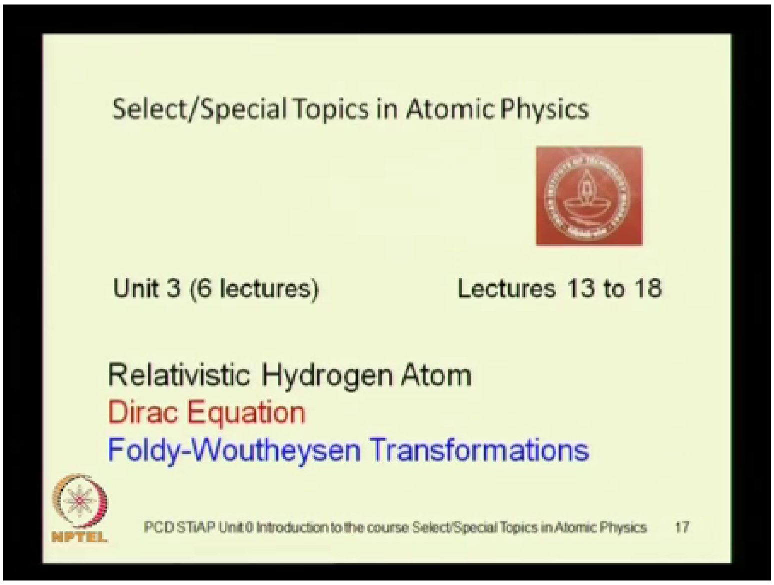

Select/Special Topics in Atomic Physics

Unit 3 (6 lectures)

Lectures 13 to 18

Relativistic Hydrogen Atom

Dirac Equation

Foldy-Woutheysen Transformations

In unit 3, we will study the relativistic hydrogen atom and this comes into play, because the speed of light is finite. And therefore, all consequences of the special theory of relativity must be accounted for and an important consequences that, space intervals and time intervals are not independently invariant under transformations, when you go for one frame to another frame, which is moving even constant of velocity with respect to an earlier frame.

So, all of consequences of the constancy, and the finite value of the speed of light in vacuum have to be accounted for… Now, what it does is, it makes us necessary to go the beyond the Schrodinger equation and for electron, you make use of the Dirac equation and then, study the consequences of the relativistic quantum mechanical equation.

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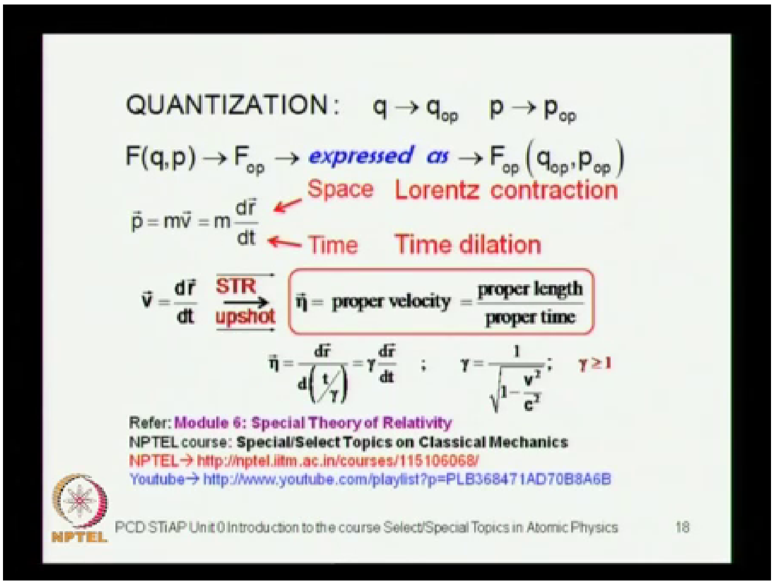

QUANTIZATION: $q \to q_{op} \quad p \to p_{op}$

$F(q,p) \to F_{op} \to$ *expressed as* $\to F_{op}\left(q_{op}, p_{op}\right)$

$\vec{p} = m\vec{v} = m\frac{d\vec{r}}{dt}$

Space Lorentz contraction

Time Time dilation

$\vec{v} = \frac{d\vec{r}}{dt} \xrightarrow[\text{upshot}]{\text{STR}} \boxed{\vec{\eta} = \text{proper velocity} = \frac{\text{proper length}}{\text{proper time}}}$

$\vec{\eta} = \frac{d\vec{r}}{d\left(t/\gamma\right)} = \gamma\frac{d\vec{r}}{dt} \quad ; \quad \gamma = \frac{1}{\sqrt{1-\frac{v^2}{c^2}}}; \quad \gamma \geq 1$

Refer: Module 6: Special Theory of Relativity

NPTEL course: Special/Select Topics on Classical Mechanics

NPTEL→ http://nptel.iitm.ac.in/courses/115106068/

Youtube→ http://www.youtube.com/playlist?p=PLB368471AD70B8A6B

PCD STiAP Unit 0 Introduction to the course Select/Special Topics in Atomic Physics 18

Now, in particular what happens is that, momentum is what you quantize in quantum mechanics. So, the operator for momentum is minus h cross radiance operator, which we would have learned in your first course. But then, what is momentum, normally you will define it as mass times the rate of change of velocity, rate of change of position. Velocity is rate of change position, so mass into velocity is the momentum. But, the numerator here and the denominator here, are not independently invariant under Lorentz transformations.

The numerator, the space intervals undergo Lorentz contractions and the time intervals undergo time dilation. So, one has to be introduce a fore momentum, one has to introduce, what is called as a proper velocity and proper momentum. So, we will go through these corrections or revisions to some of the classical ideas in non relativistic classical mechanics. They are important also in classical relativistic mechanics, which is does not involve quantum phenomenon, even there these things are important. But, in particular, they will be of significance to ask in the contest of quantum mechanics.

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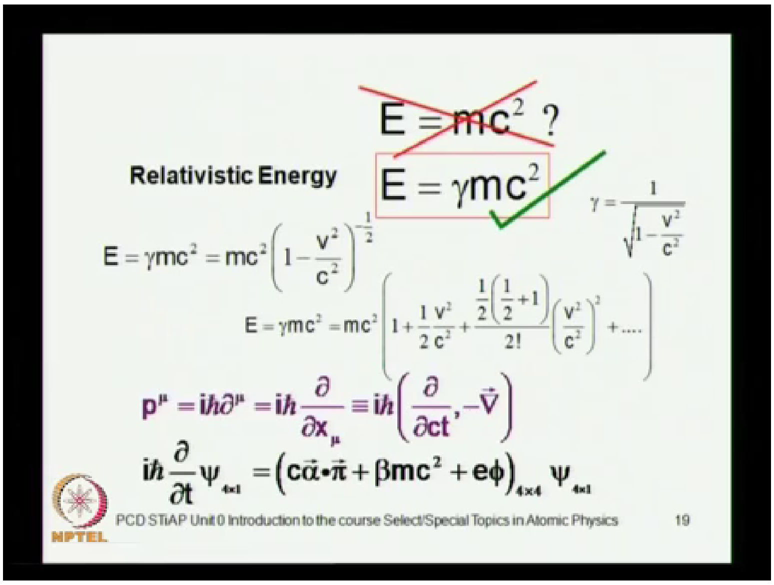

$$\cancel{E = mc^2}\ ?$$

Relativistic Energy

$$\boxed{E = \gamma mc^2} \checkmark$$

$$\gamma = \frac{1}{\sqrt{1-\frac{v^2}{c^2}}}$$

$$E = \gamma mc^2 = mc^2\left(1-\frac{v^2}{c^2}\right)^{-\frac{1}{2}}$$

$$E = \gamma mc^2 = mc^2\left(1+\frac{1}{2}\frac{v^2}{c^2}+\frac{\frac{1}{2}\left(\frac{1}{2}+1\right)}{2!}\left(\frac{v^2}{c^2}\right)^2+\ldots.\right)$$

$$p^\mu = i\hbar\partial^\mu = i\hbar\frac{\partial}{\partial x_\mu} \equiv i\hbar\left(\frac{\partial}{\partial ct},-\vec{\nabla}\right)$$

$$i\hbar\frac{\partial}{\partial t}\psi_{4\times1} = \left(c\vec{\alpha}\bullet\vec{\pi}+\beta mc^2+e\phi\right)_{4\times4}\psi_{4\times1}$$

PCD STiAP Unit 0 Introduction to the course Select/Special Topics in Atomic Physics 19

So, in the process we will also learn, what is the correct expression for the relativistic energy of a particle. And then, we will proceed to quantize the system by having a appropriate operator in place of dynamical variables and we will arrive at the frame is Dirac equation, which you see at the bottom. Now, this Dirac equation of course, has some very important consequences, when you set it for the electron you find that, it assigns to the electron an additional integral property, which is integral to the presence of the electron and this is the intrinsic angular momentum of the electron. Now, this can couple to the orbital angular momentum and that is the famous spin orbit coupling. But, where is the spin orbit interactions s dot l in the Dirac equation, you do not see it in the form, in which you see the Dirac equation in front of you.

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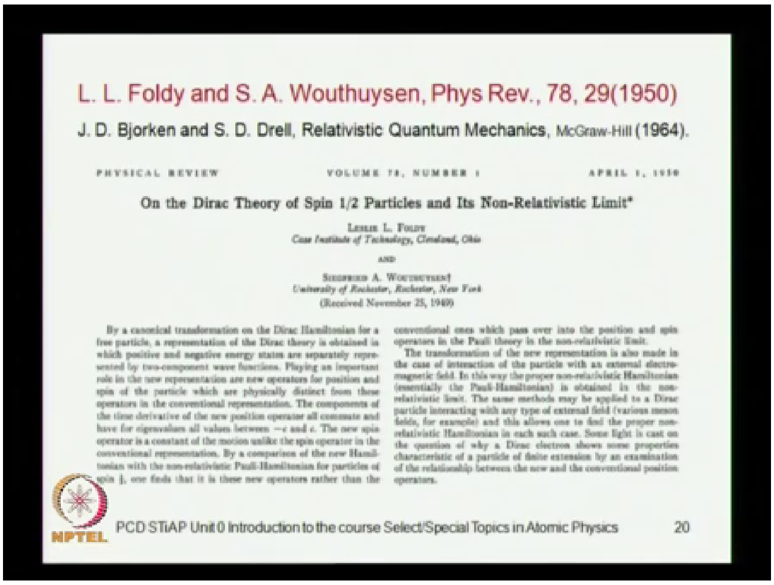

L. L. Foldy and S. A. Wouthuysen, Phys Rev., 78, 29(1950)

J. D. Bjorken and S. D. Drell, Relativistic Quantum Mechanics, McGraw-Hill (1964).

PHYSICAL REVIEW VOLUME 78, NUMBER 1 APRIL 1, 1950

On the Dirac Theory of Spin 1/2 Particles and Its Non-Relativistic Limit*

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AND

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(Received November 25, 1949)

PCD STiAP Unit 0 Introduction to the course Select/Special Topics in Atomic Physics 20

But, what you can do is subject, the Dirac equation to a number of transformations, which are known as the Foldy Woutheysen transformations. And we will discuss this paper to some extant in this unit that, this is the procedure to transform the Dirac equation to different representations. And you go through a series of representation called as the Foldy Woutheysen's first representation, the second representation and third representation. And when you go through these different Foldy Woutheysen representations, you arrive at a form of the Dirac equation, which is completely based on Dirac equation.

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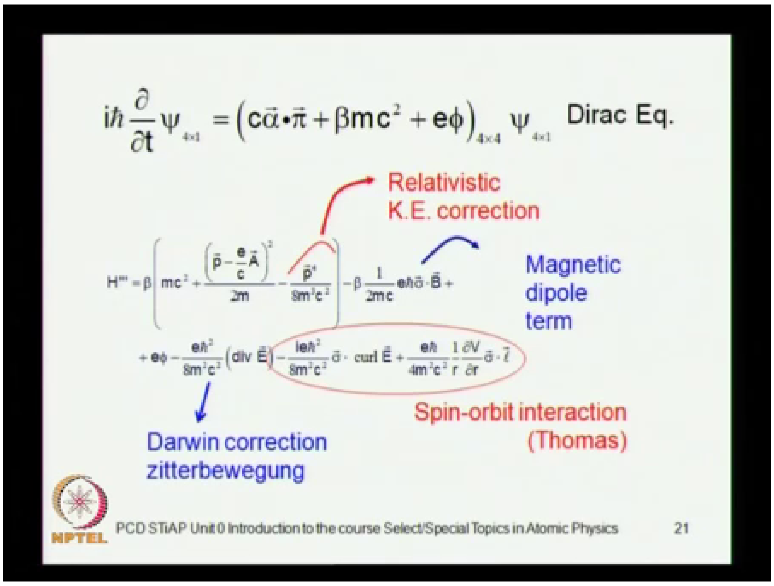

$$i\hbar\frac{\partial}{\partial t}\psi_{4\times1}=\left(c\vec{\alpha}\bullet\vec{\pi}+\beta mc^2+e\phi\right)_{4\times4}\psi_{4\times1}$$ Dirac Eq.

$$H'''=\beta\left(mc^2+\frac{\left(\vec{p}-\frac{e}{c}\vec{A}\right)^2}{2m}-\frac{\vec{p}^4}{8m^3c^2}\right)-\beta\frac{1}{2mc}e\hbar\vec{\sigma}\cdot\vec{B}+$$

$$+e\phi-\frac{e\hbar^2}{8m^2c^2}\left(\operatorname{div}\vec{E}\right)-\frac{ie\hbar^2}{8m^2c^2}\vec{\sigma}\cdot\operatorname{curl}\vec{E}+\frac{e\hbar}{4m^2c^2}\frac{1}{r}\frac{\partial V}{\partial r}\vec{\sigma}\cdot\vec{l}$$

Relativistic K.E. correction

Magnetic dipole term

Spin-orbit interaction (Thomas)

Darwin correction zitterbewegung

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But then, it attains a form, in which the Hamiltonian has got these terms and you can recognize clearly, what are the terms which are responsible for the relativistic kinetic energy correction or the spin orbit interaction and so on. So, all of these terms, which are already there in the Dirac equation, they become manifest. So, Foldy Woutheysen transformation is really an extremely important one to get into the hard of physics, which is coming out to the Dirac equation, so we will discuss this in some details in this unit.

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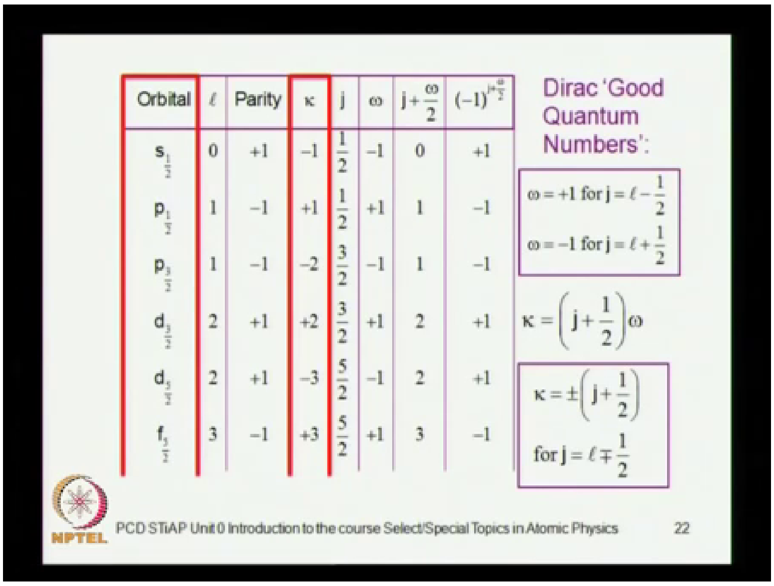

Orbital	ℓ	Parity	κ	j	ω	$j+\frac{\omega}{2}$	$(-1)^{j+\frac{\omega}{2}}$
$s_{\frac{1}{2}}$	0	+1	−1	$\frac{1}{2}$	−1	0	+1
$p_{\frac{1}{2}}$	1	−1	+1	$\frac{1}{2}$	+1	1	−1
$p_{\frac{3}{2}}$	1	−1	−2	$\frac{3}{2}$	−1	1	−1
$d_{\frac{3}{2}}$	2	+1	+2	$\frac{3}{2}$	+1	2	+1
$d_{\frac{5}{2}}$	2	+1	−3	$\frac{5}{2}$	−1	2	+1
$f_{\frac{5}{2}}$	3	−1	+3	$\frac{5}{2}$	+1	3	−1

Dirac 'Good Quantum Numbers':

$\omega = +1$ for $j = \ell - \frac{1}{2}$

$\omega = -1$ for $j = \ell + \frac{1}{2}$

$$\kappa = \left(j + \frac{1}{2}\right)\omega$$

$$\kappa = \pm\left(j + \frac{1}{2}\right)$$

for $j = \ell \mp \frac{1}{2}$

We will also learn about, what are the good quantum numbers for Dirac electron, so in particular, we will discuss the kappa quantum number.

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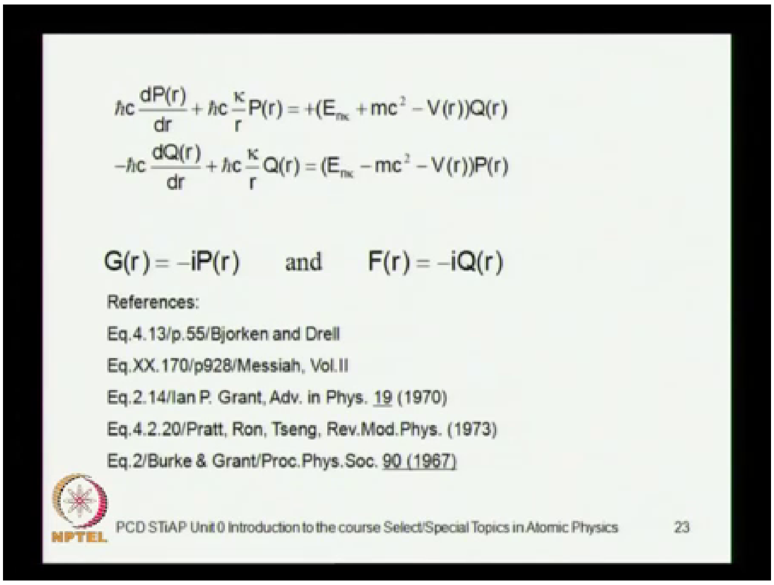

$$\hbar c\frac{dP(r)}{dr}+\hbar c\frac{\kappa}{r}P(r)=+(E_{n\kappa}+mc^2-V(r))Q(r)$$

$$-\hbar c\frac{dQ(r)}{dr}+\hbar c\frac{\kappa}{r}Q(r)=(E_{n\kappa}-mc^2-V(r))P(r)$$

$$G(r)=-iP(r) \quad \text{and} \quad F(r)=-iQ(r)$$

References:

Eq.4.13/p.55/Bjorken and Drell

Eq.XX.170/p928/Messiah, Vol.II

Eq.2.14/Ian P. Grant, Adv. in Phys. 19 (1970)

Eq.4.2.20/Pratt, Ron, Tseng, Rev.Mod.Phys. (1973)

Eq.2/Burke & Grant/Proc.Phys.Soc. 90 (1967)

And then, we will proceed to get the radial coupled equations for the large part in the small part of the wave function in the Dirac equation. And the motivation to do this is to ((Refer Time: 19:18)) with some of the preliminary tools that are required to read about relativistic atomic physics. Because, anything in relativistic, anything in atomic physics will begin with wave functions and quantum numbers and so on, and the appropriate quantum numbers and wave functions are of course, the relativistic ones.

Because, nature does obey relativistic quantum mechanics more so than the non relativistic quantum mechanics, for the simple reason that, laws of nature are determine also by the finite speed of light. So, if you want to read any of these articles, which are the most common literature or other papers also, which was equivalent to them in some sense and they will give you a short and you will get sort of any introduction to the terminology and methodology of quantum mechanics, which is used in literature. So, you will get some introduction into that, as a result of this unit.

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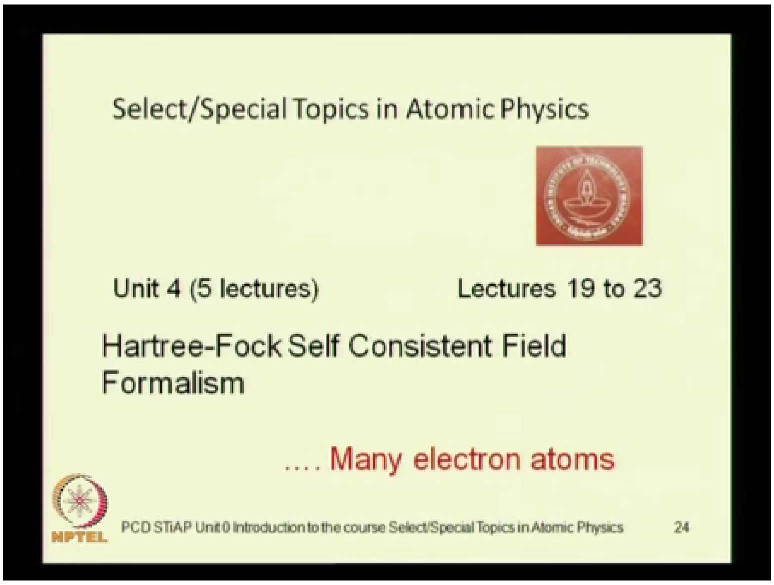

Select/Special Topics in Atomic Physics

Unit 4 (5 lectures) Lectures 19 to 23

Hartree-Fock Self Consistent Field Formalism

.... Many electron atoms

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Then, in unit 4, we will have 5 classes on many electron items and the method to deal with many electron atoms comes from Hartree, further developed by Fock and Slater, and some others.

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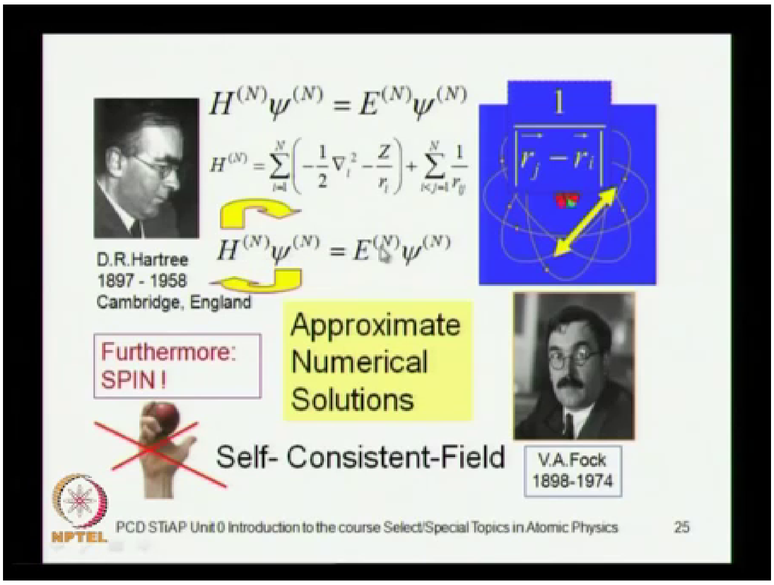

$$H^{(N)}\psi^{(N)} = E^{(N)}\psi^{(N)}$$

$$H^{(N)} = \sum_{i=1}^{N}\left(-\frac{1}{2}\nabla_i^2 - \frac{Z}{r_i}\right) + \sum_{i<j=1}^{N}\frac{1}{r_{ij}}$$

$$\frac{1}{\left|\vec{r}_j - \vec{r}_i\right|}$$

$$H^{(N)}\psi^{(N)} = E^{(N)}\psi^{(N)}$$

D.R.Hartree
1897 - 1958
Cambridge, England

Furthermore: SPIN !

Approximate Numerical Solutions

Self- Consistent-Field

V.A.Fock
1898-1974

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And basically, it addresses the CATCH 22 kind of situation that, to set up this Schrodinger equation for the n electronic system, H psi equal to E psi for the n electrons, you need of course, the Hamiltonian. So that, you can set up, you can solve the differential equation and get the solutions but then, to be able to set up the Hamiltonian itself, you need the solution in advance.

And this is a situation, which needs to be addressed and using methods, which were developed by Hartree and then, further there were contributions to include the electron spin by Fock and Slater. This is the method which is known as Hartree Fock method, so we will discuss the self consistent field method of developed by Hartree Fock.

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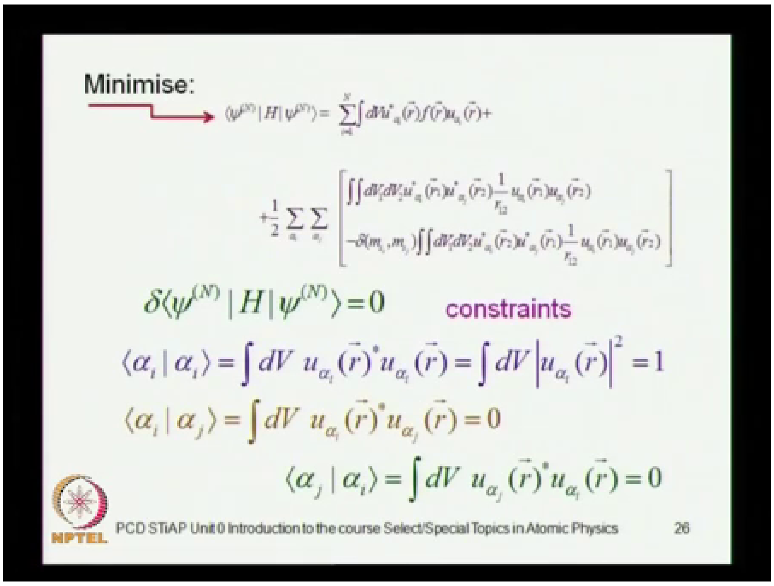

Minimise:

$$\xrightarrow{} \langle\psi^{(N)}|H|\psi^{(N)}\rangle = \sum_{i=1}^{N}\int dV u^*_{\alpha_i}(\vec{r}) f(\vec{r}) u_{\alpha_i}(\vec{r}) +$$

$$+\frac{1}{2}\sum_{\alpha_i}\sum_{\alpha_j}\begin{bmatrix}\iint dV_1 dV_2 u^*_{\alpha_i}(\vec{r}_1) u^*_{\alpha_j}(\vec{r}_2)\frac{1}{r_{12}}u_{\alpha_i}(\vec{r}_1)u_{\alpha_j}(\vec{r}_2)\\ -\delta(m_{s_i},m_{s_j})\iint dV_1 dV_2 u^*_{\alpha_i}(\vec{r}_2) u^*_{\alpha_j}(\vec{r}_1)\frac{1}{r_{12}}u_{\alpha_i}(\vec{r}_1)u_{\alpha_j}(\vec{r}_2)\end{bmatrix}$$

$$\delta\langle\psi^{(N)}|H|\psi^{(N)}\rangle = 0$$

constraints

$$\langle\alpha_i|\alpha_i\rangle = \int dV\, u_{\alpha_i}(\vec{r})^* u_{\alpha_i}(\vec{r}) = \int dV \left|u_{\alpha_i}(\vec{r})\right|^2 = 1$$

$$\langle\alpha_i|\alpha_j\rangle = \int dV\, u_{\alpha_i}(\vec{r})^* u_{\alpha_j}(\vec{r}) = 0$$

$$\langle\alpha_j|\alpha_i\rangle = \int dV\, u_{\alpha_j}(\vec{r})^* u_{\alpha_i}(\vec{r}) = 0$$

NPTEL PCD STiAP Unit 0 Introduction to the course Select/Special Topics in Atomic Physics 26

And in this, the problem is, addressed using a variations techniques, in which one minimizes or gets the extremum of the expectation value of the Hamiltonian in n electron quantum mechanical state of the system. And this n electron state must be properly antisymmetrized, because the electrons are fermions. And using a properly antisymmetrized n electron state, you obtained a variation of extremum of the Hamiltonian, subject to certain constraints that, the variation of remain orthogonal to each other and they are also normalized. So, subject to these constraints, you get variation solutions.

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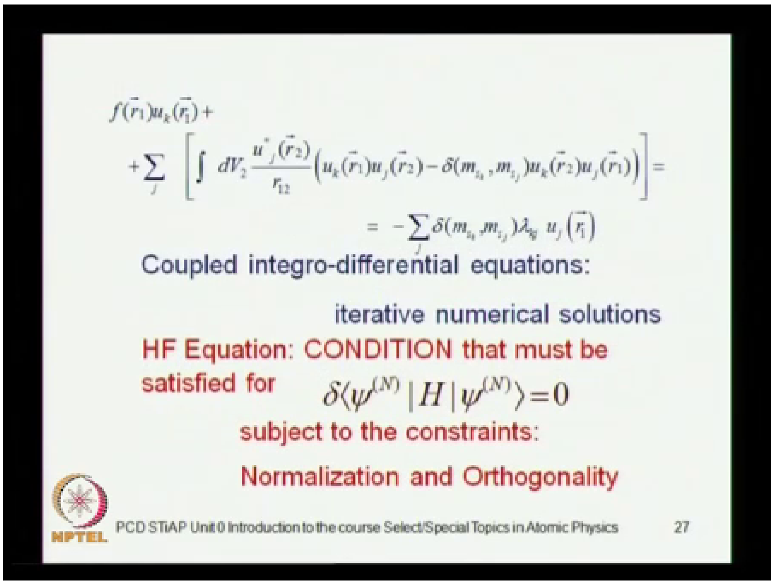

$$f(\vec{r}_1)u_k(\vec{r}_1)+$$
$$+\sum_j\left[\int dV_2\frac{u^*_j(\vec{r}_2)}{r_{12}}\Big(u_k(\vec{r}_1)u_j(\vec{r}_2)-\delta(m_{s_k},m_{s_j})u_k(\vec{r}_2)u_j(\vec{r}_1)\Big)\right]=$$
$$=-\sum_j\delta(m_{s_k},m_{s_j})\lambda_{kj}\,u_j(\vec{r}_1)$$

Coupled integro-differential equations:

iterative numerical solutions

HF Equation: CONDITION that must be satisfied for $\delta\langle\psi^{(N)}|H|\psi^{(N)}\rangle=0$

subject to the constraints:

Normalization and Orthogonality

PCD STiAP Unit 0 Introduction to the course Select/Special Topics in Atomic Physics 27

They give you a certain set of coupled integral differential equations, which are called Hartree Fock equations. And essentially, this equation emerges as a condition that must be satisfied so that, you get self consistent field solution. So, it is a condition, which merges from this analysis from the variation tool so that, the constraints are respected and you get an extremum in the expectation value of the Hamiltonian. So, this is the Hartree Fock equation that we will develop in this unit.

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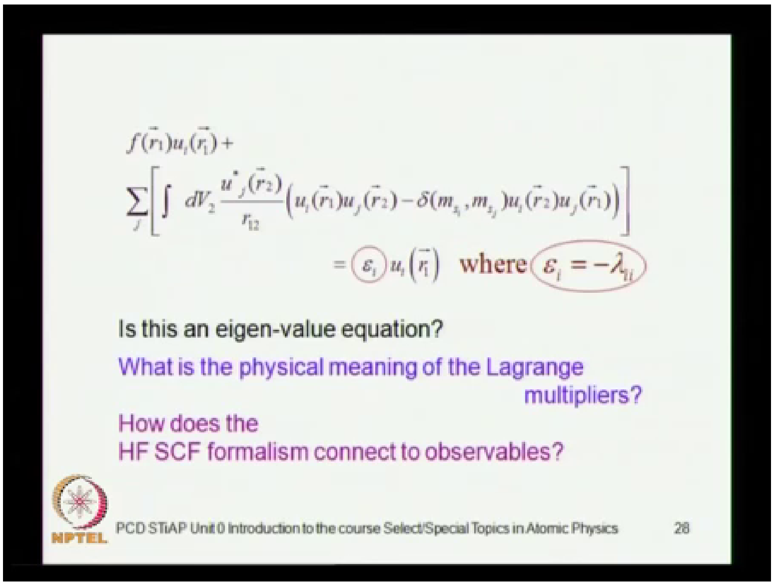

$$f(\vec{r}_1)u_i(\vec{r}_1)+$$
$$\sum_j\left[\int dV_2\frac{u^*_j(\vec{r}_2)}{r_{12}}\Big(u_i(\vec{r}_1)u_j(\vec{r}_2)-\delta(m_{s_i},m_{s_j})u_i(\vec{r}_2)u_j(\vec{r}_1)\Big)\right]$$
$$=\boxed{\varepsilon_i}\,u_i(\vec{r}_1)\quad\text{where}\ \boxed{\varepsilon_i=-\lambda_{ii}}$$

Is this an eigen-value equation?

What is the physical meaning of the Lagrange multipliers?

How does the HF SCF formalism connect to observables?

PCD STiAP Unit 0 Introduction to the course Select/Special Topics in Atomic Physics 28

We will also explicit in, what is called as the Hartree Fock equation in the diagonal form and this is a very powerful frame work. Because, it tells us that, the variational parameter which are introduced through via the method of Lagrangious method of variation multipliers, they acquire a very specific physical meaning, which is amenable to measurements. So, it connects the Hartree Fock theory to physical measurements directly, because the energy values which appear in the Hartree Fock equation in the diagonal form are then, associated with binding energies, which are measurable like ionization potential. So, you can carry out some measurements and actually connect them.

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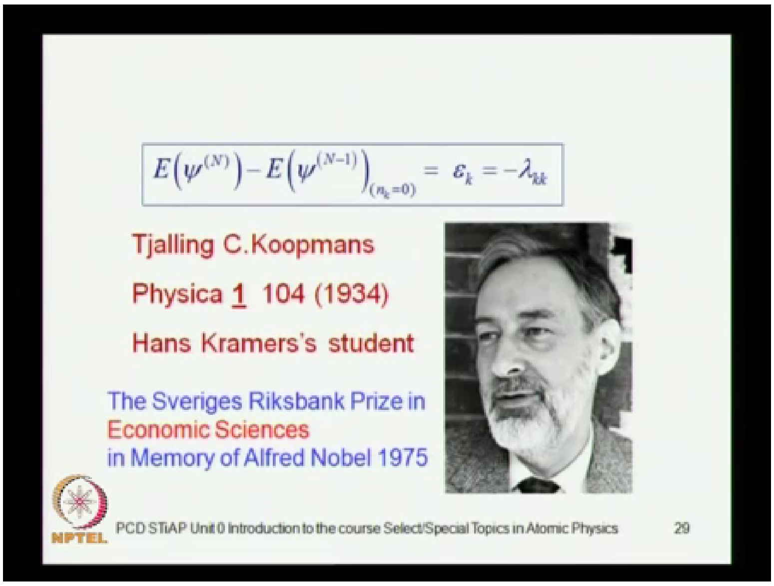

$$\boxed{E\left(\psi^{(N)}\right)-E\left(\psi^{(N-1)}\right)_{(n_k=0)} = \varepsilon_k = -\lambda_{kk}}$$

Tjalling C.Koopmans

Physica 1 104 (1934)

Hans Kramers's student

The Sveriges Riksbank Prize in
Economic Sciences
in Memory of Alfred Nobel 1975

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So, there is very famous theorem which does this, which is known as the Koopmans theorem, which we will derive and prove, and we will establish this. So, it tells you that, the energy difference between n electron state and n minus 1 electrons state gives you the energy value that appears in the Hartree Fock equation in the diagonal form. So, that is the Koopmans theorem, which we will discuss.

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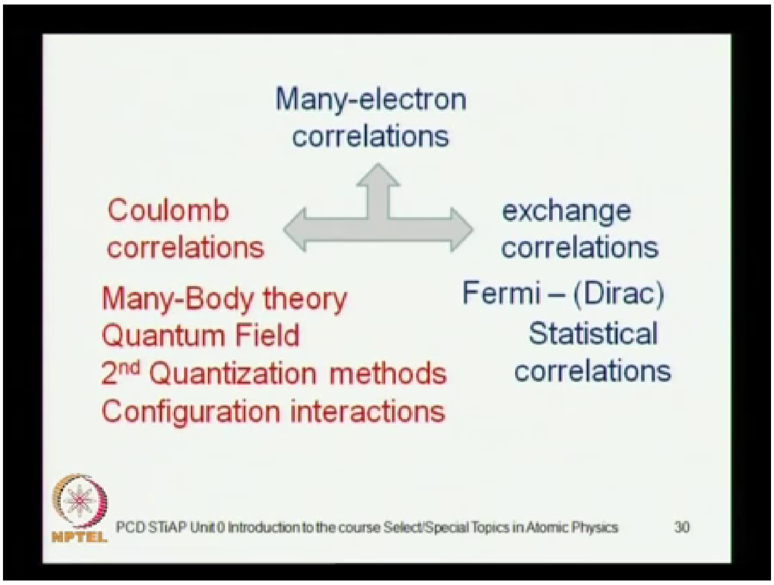

Many-electron correlations

Coulomb correlations

exchange correlations

Many-Body theory
Quantum Field
2nd Quantization methods
Configuration interactions

Fermi – (Dirac) Statistical correlations

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But, this remains valid in an approximation. which is called as independent practical approximation, because Zeeman effects takes into account the electron electron interaction 1 over r by r i j, it does leave out what is called as electron electron correlation. And there are two kinds of correlations, one is exchange correlations or the statistical correlations coming from the electron spin and there are other correlations, which are known as coulomb correlations.

And the coulomb correlations require many body field theoretical methods, second quantization methods, configuration interaction methods and so on. So, one requires some further quantum mechanics would develop this, which will go beyond the scope of this course. But, I will certainly mention that, this is what provides the frame work for the fundamental Hartree Fock.

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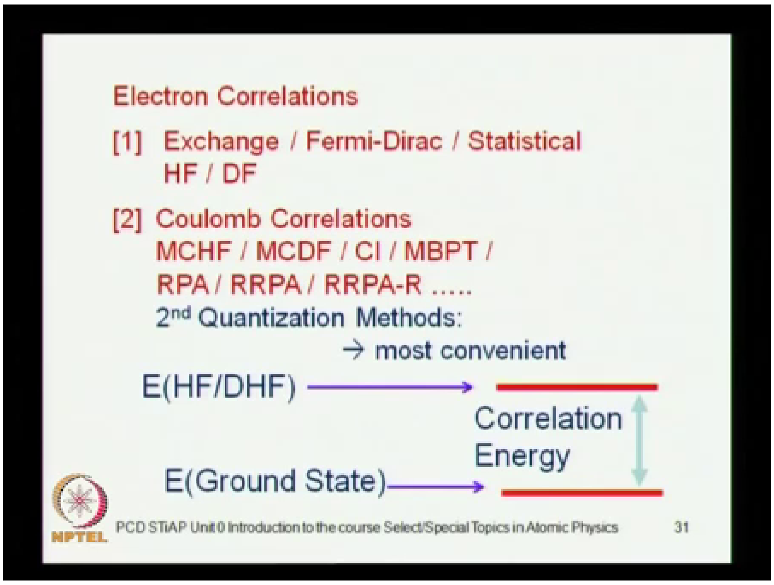

Electron Correlations

[1] Exchange / Fermi-Dirac / Statistical
HF / DF

[2] Coulomb Correlations
MCHF / MCDF / CI / MBPT /
RPA / RRPA / RRPA-R .....
2^{nd} Quantization Methods:
→ most convenient

E(HF/DHF) →

Correlation Energy

E(Ground State) →

Of course, one can extended to, what is called as a multiple configuration Hartree Fock or if you do a relativistic coefficient, you get what is called as the multi configuration Dirac Fock. There are other methods of dealing with electron correlations like the random phase approximation, the relativistic correlation, relativistic random phase approximation and so on. So, there are you know, one can go a long way but then, the Hartree Fock of the Dirac Hartree Fock restricts you to, it enables you to accommodate the statistical and the exchange correlations, but it leaves out the coulomb correlations. So, that is the difference and limitation of the Hartree Fock and Dirac Fock method.

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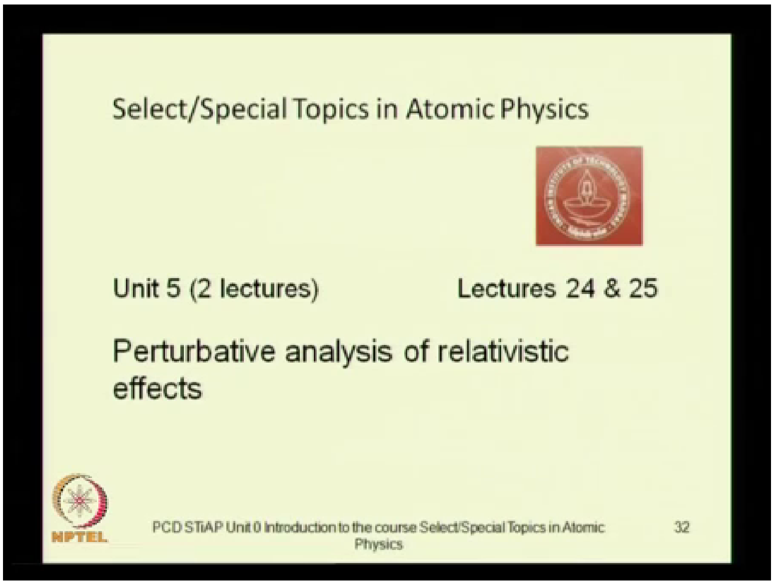

Select/Special Topics in Atomic Physics

Unit 5 (2 lectures) Lectures 24 & 25

Perturbative analysis of relativistic effects

Then, in unit 5, which will be a tiny unit, just two classes in this, we will deal with perturbative analysis of the relativistic effects. So, we would have already consider the relativistic effects in our earlier unit on Dirac equation and Foldy Woutheysen transformations.

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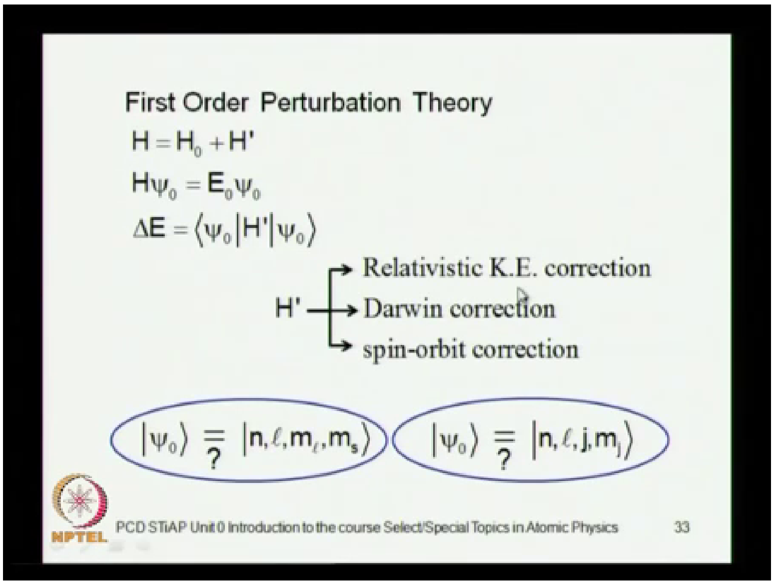

First Order Perturbation Theory

$H = H_0 + H'$

$H\psi_0 = E_0\psi_0$

$\Delta E = \langle \psi_0 | H' | \psi_0 \rangle$

H' → Relativistic K.E. correction
H' → Darwin correction
H' → spin-orbit correction

$|\psi_0\rangle \underset{?}{=} |n,\ell,m_\ell,m_s\rangle$

$|\psi_0\rangle \underset{?}{=} |n,\ell,j,m_j\rangle$

PCD STiAP Unit 0 Introduction to the course Select/Special Topics in Atomic Physics 33

But, in this unit we will see that, if you look at these individual corrections, you can think of these terms as correction to the non relativistic problem or as additional factor has to be taken into account. And you take them into an account piece wise, like you can plug in the relativistic kinetic energy correction, you can plug in the Darwin connection and you can plug in the spin orbit correction. And you can get these corrections using first order perturbation theory or even higher order perturbation theory if you like, in which the energy correction is given by the expectation value of the perturbation Hamiltonian in the unperturbed state. But then, the question arises as to what are the appropriated bases such to be used and this is an important question, which we will discuss in this unit.

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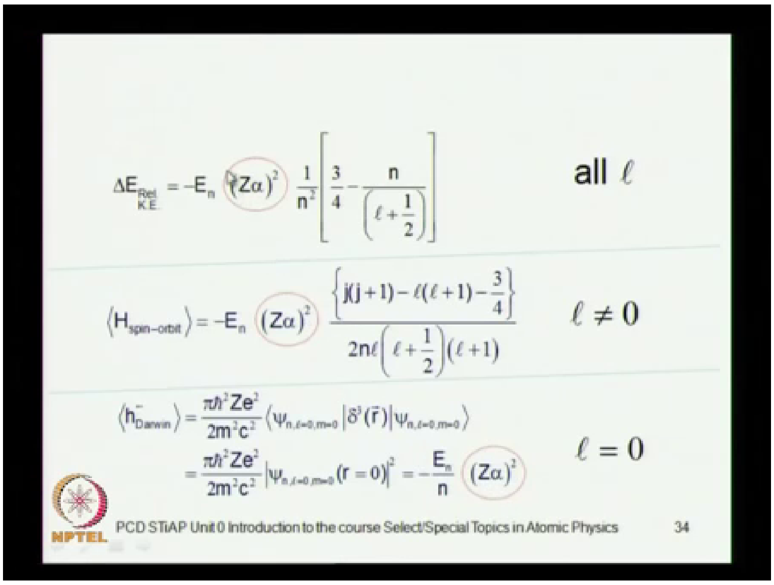

$$\Delta E_{\substack{\text{Rel}\\ \text{K.E.}}} = -E_n (Z\alpha)^2 \frac{1}{n^2}\left[\frac{3}{4} - \frac{n}{\left(\ell+\frac{1}{2}\right)}\right]$$

all ℓ

$$\left\langle H_{\text{spin-orbit}} \right\rangle = -E_n (Z\alpha)^2 \frac{\left\{j(j+1) - \ell(\ell+1) - \frac{3}{4}\right\}}{2n\ell\left(\ell+\frac{1}{2}\right)(\ell+1)}$$

$\ell \neq 0$

$$\left\langle h_{\text{Darwin}}^{-} \right\rangle = \frac{\pi\hbar^2 Ze^2}{2m^2c^2}\left\langle \psi_{n,\ell=0,m=0}\left|\delta^3(\vec{r})\right|\psi_{n,\ell=0,m=0}\right\rangle$$

$$= \frac{\pi\hbar^2 Ze^2}{2m^2c^2}\left|\psi_{n,\ell=0,m=0}(r=0)\right|^2 = -\frac{E_n}{n}(Z\alpha)^2$$

$\ell = 0$

And you will find that, if you look at the corrections due to the relativistic kinetic energy term or the spin orbit term or Darwin term, they are all of the same order of magnitude, they are all of the corrections are go as Z alpha square, where alpha is a fine structure constant, Z is the atomic number, so they all equally important and notice that, they all depend on the value of l in some way. So, if you did only this correction, but not the other two, you will get n l dependent answer.

But, the final Dirac solution, which we have already got, which we would have already got in unit 3, in fact would tell us that, the Dirac energy is depend only on the j value and they are independent on the l value. So, only when you put all of these three corrections together you find that, the dependence of energy is only on j and not on l quantum numbers. So, how it this to be treated pertubativly, what are the appropriate unperturbed stage, which must be used to get the corresponding perturbative corrections, so this will be the subject of this unit.

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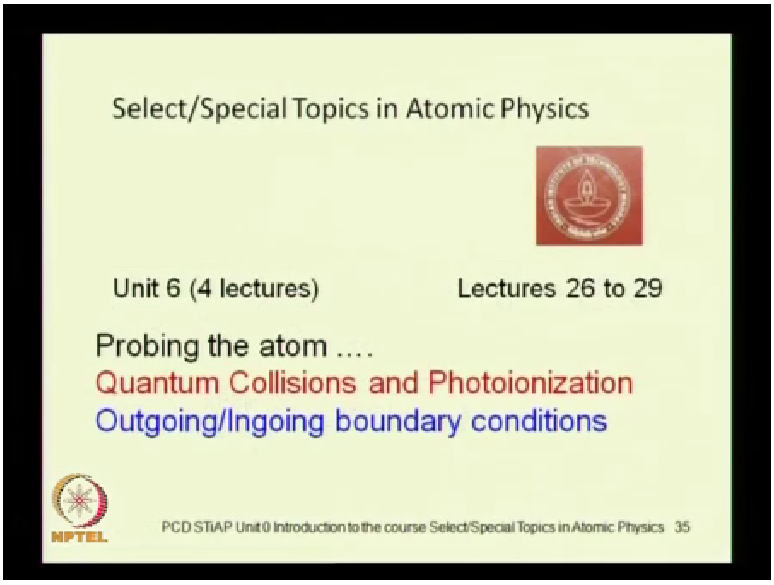

Select/Special Topics in Atomic Physics

Unit 6 (4 lectures) Lectures 26 to 29

Probing the atom ….

Quantum Collisions and Photoionization

Outgoing/Ingoing boundary conditions

PCD STiAP Unit 0 Introduction to the course Select/Special Topics in Atomic Physics 35

And then, unit 6, we will discuss, how an atom is probed and to probing the atom, you need some tools, something which will come and interact with the atom.

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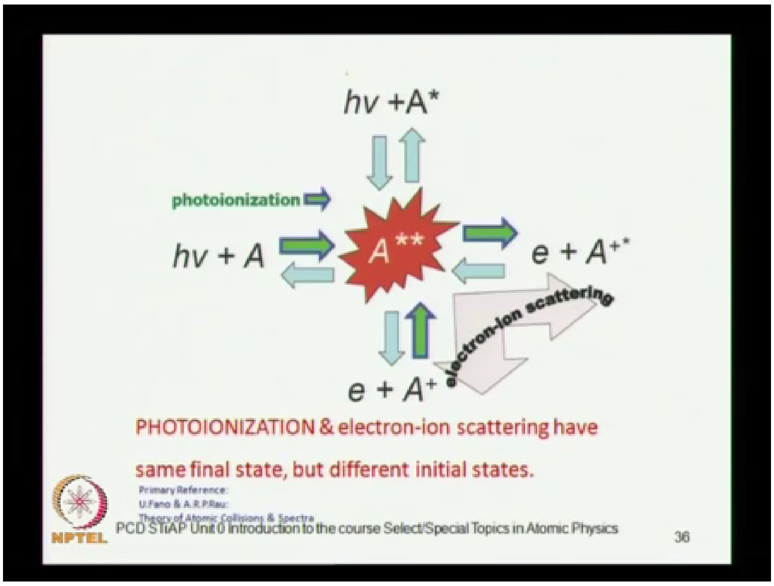

PHOTOIONIZATION & electron-ion scattering have same final state, but different initial states.

Primary Reference:
U.Fano & A.R.P.Rau:
Theory of Atomic Collisions & Spectra

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And the kinds of probe that you can think of are, either particles like electrons you can have, you can fire electrons coming out of an electron gun at an atom and see the scattering, so this can be one way probing the atom. Another way of probing an atom could be to shine light on it and see, how the atom response to this light. So, there are these alternate tools that are available to you like photo ionization or electron scattering and so on.

And you recognize from this figure that, if you go from left or right in this figure, that you got a photon, which is observed by an atom giving you an electron and an ion in the final state. This is the same state that you can get, if you had completely different ingredients in the initial stage. That if you want to have an electron ion scattering experiments, again you can get electron and an ion in the final stage. So, which means, that for the same final state, you can have completely different pears of ingredients.

In this case, you have got electron and an ion, in this case you have got a photon and a neutral atom. So, obviously, one expects some sort of connection between these two processes and indeed, there is such a connection, which allows you to develop the techniques in one field in scattering theory for example, and use them in photo ionization and vice-a-versa. So, basically both photo ionization and scattering, they are two aspects of the same quantum mechanics. And there is no real fundamental difference between scattering and spectroscopy.

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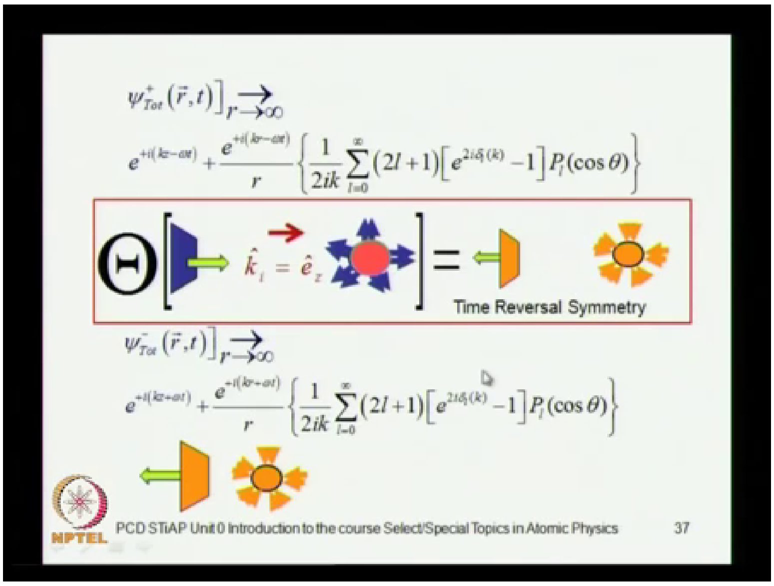

$$\psi^{+}_{Tot}(\vec{r},t)\Big]_{r\to\infty} \rightarrow$$

$$e^{+i(kz-\omega t)} + \frac{e^{+i(kr-\omega t)}}{r}\left\{\frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)\left[e^{2i\delta_l(k)}-1\right]P_l(\cos\theta)\right\}$$

$$\Theta\left[\quad \hat{k}_i = \hat{e}_z \quad\right] =$$

Time Reversal Symmetry

$$\psi^{-}_{Tot}(\vec{r},t)\Big]_{r\to\infty} \rightarrow$$

$$e^{+i(kz+\omega t)} + \frac{e^{+i(kr+\omega t)}}{r}\left\{\frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)\left[e^{2i\delta_l(k)}-1\right]P_l(\cos\theta)\right\}$$

PCD STiAP Unit 0 Introduction to the course Select/Special Topics in Atomic Physics 37

So, the relationship is governed by, what is called as the time reversal symmetry in quantum mechanics that, if you have electron and an atom in or a target in the initial state, how you can subject this to a time reversal process. And this time reversal process in quantum mechanics is not just t going to minus t, you have to take into account some additional factors, which we will discuss applying in this unit. And we will find that, photo ionization and the electron ion scattering solutions are connected by the time reversal symmetry.

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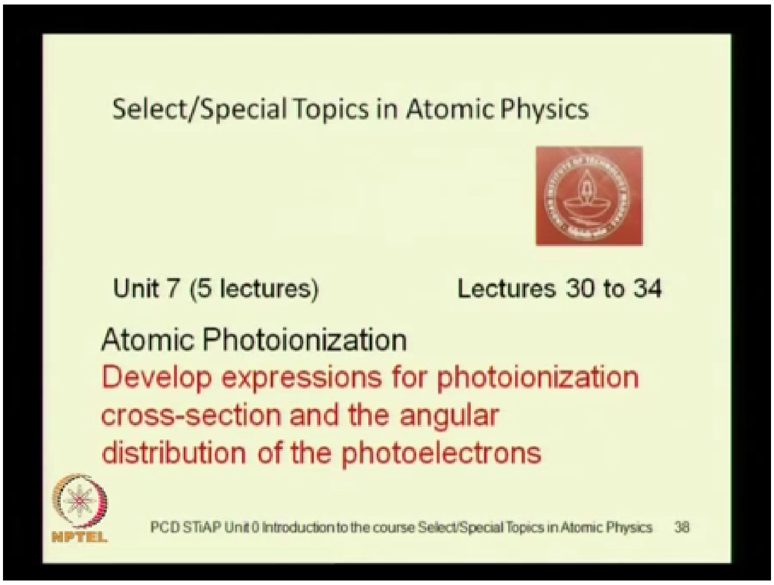

Select/Special Topics in Atomic Physics

Unit 7 (5 lectures) Lectures 30 to 34

Atomic Photoionization

Develop expressions for photoionization cross-section and the angular distribution of the photoelectrons

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This is important, because it will give you the boundary condition, which are appropriate for the two processes. And you must use the wave functions with the correct boundary conditions so that, you can apply this and get other things like matrix elements, the photo ionization cross sections, angular distribution of the photo electrons and so on. And this is what we will study in unit 7, in which we will need the continuum final state solution with appropriate boundary conditions namely, what are known as ingoing wave boundary conditions. So, the different between the ingoing wave boundary condition and outgoing boundary conditions is, what we will study in unit 6.

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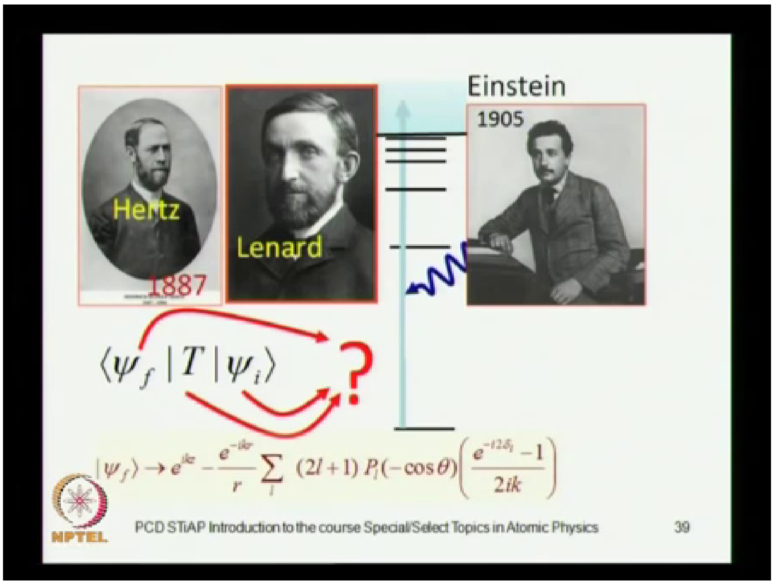

$$\langle\psi_f\,|\,T\,|\,\psi_i\rangle$$

$$|\psi_f\rangle \to e^{ikz} - \frac{e^{-ikr}}{r}\sum_l (2l+1)\,P_l(-\cos\theta)\left(\frac{e^{-i2\delta_l}-1}{2ik}\right)$$

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And in unit 7, we will apply them to the study of atomic photo ionization, in which we will use the wave function, further final state of appropriate boundary conditions in a photo ionization experiment.

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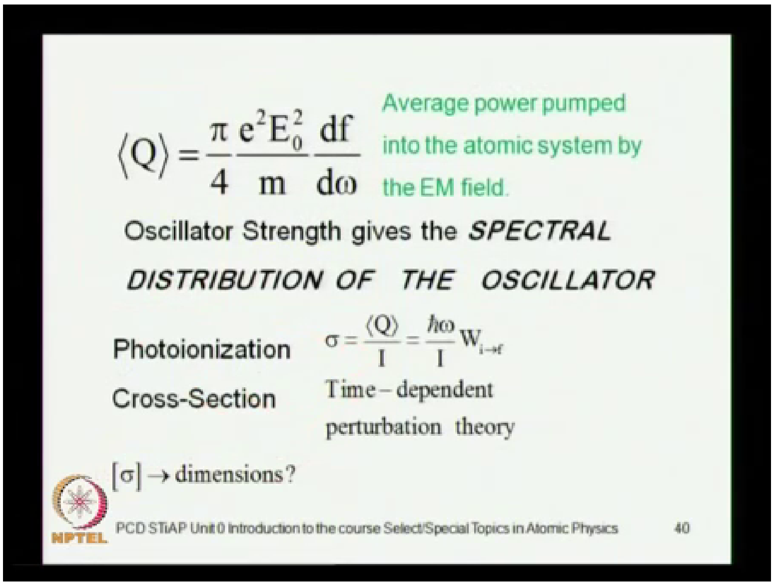

$$\langle Q \rangle = \frac{\pi}{4}\frac{e^2E_0^2}{m}\frac{df}{d\omega}$$

Average power pumped into the atomic system by the EM field.

Oscillator Strength gives the ***SPECTRAL DISTRIBUTION OF THE OSCILLATOR***

Photoionization Cross-Section $\sigma = \frac{\langle Q \rangle}{I} = \frac{\hbar\omega}{I} W_{i\to f}$

Time – dependent perturbation theory

$[\sigma] \to$ dimensions ?

And then, get the correct expressions for the oscillator strengths, photo ionization cross sections. And we will also in the process define, what is meant by oscillator strength, what is the classical idea of oscillator strength, what is the quantum mechanical idea of an oscillator strength.

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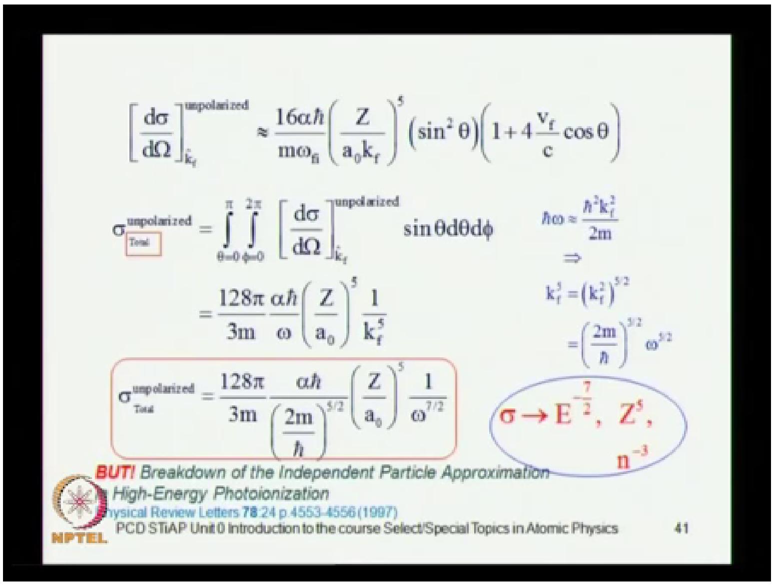

$$\left[\frac{d\sigma}{d\Omega}\right]_{\hat{k}_f}^{\text{unpolarized}} \approx \frac{16\alpha\hbar}{m\omega_{fi}}\left(\frac{Z}{a_0k_f}\right)^5 \left(\sin^2\theta\right)\left(1+4\frac{v_f}{c}\cos\theta\right)$$

$$\sigma_{\boxed{\text{Total}}}^{\text{unpolarized}} = \int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}\left[\frac{d\sigma}{d\Omega}\right]_{\hat{k}_f}^{\text{unpolarized}} \sin\theta d\theta d\phi$$

$$= \frac{128\pi}{3m}\frac{\alpha\hbar}{\omega}\left(\frac{Z}{a_0}\right)^5\frac{1}{k_f^5}$$

$$\hbar\omega \approx \frac{\hbar^2k_f^2}{2m} \Rightarrow k_f^5 = \left(k_f^2\right)^{5/2} = \left(\frac{2m}{\hbar}\right)^{5/2}\omega^{5/2}$$

$$\boxed{\sigma_{\text{Total}}^{\text{unpolarized}} = \frac{128\pi}{3m}\frac{\alpha\hbar}{\left(\frac{2m}{\hbar}\right)^{5/2}}\left(\frac{Z}{a_0}\right)^5\frac{1}{\omega^{7/2}}}$$

$$\sigma \to E^{-\frac{7}{2}},\ Z^5,\ n^{-3}$$

***BUT!** Breakdown of the Independent Particle Approximation*

High-Energy Photoionization

ysical Review Letters 78:24 p.4553-4556 (1997)

And get the estimate from the cross section we will find that, at least to a very good approximation, which is called as born approximation. The photo ionization cross section goes, it reduces with an energy, but it reduces as e to the minus 7 by 2 power of an energy and it also goes as Z to the 5, as n to the minus 3 and so on. So, these are very important results in quantum mechanics and these will be arrived in this particular unit.

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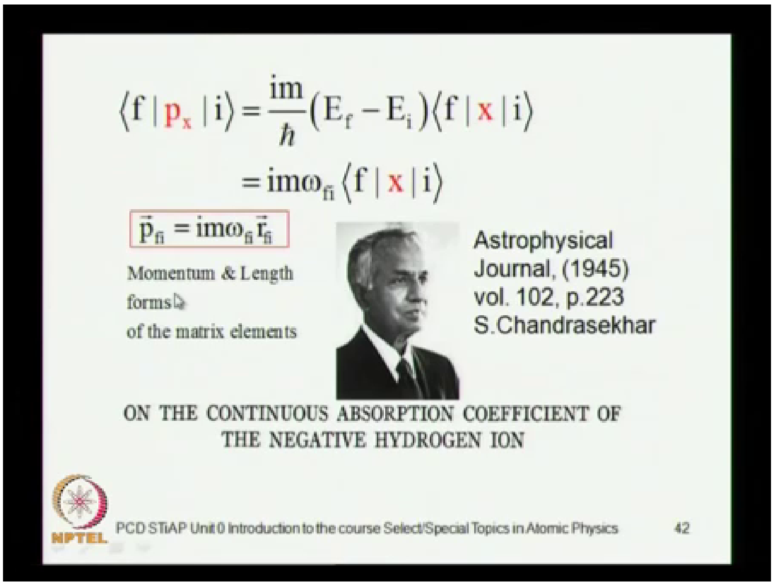

$$\langle f | p_x | i \rangle = \frac{im}{\hbar}(E_f - E_i)\langle f | x | i \rangle$$

$$= im\omega_{fi}\langle f | x | i \rangle$$

$$\boxed{\vec{p}_{fi} = im\omega_{fi}\vec{r}_{fi}}$$

Momentum & Length forms of the matrix elements

Astrophysical Journal, (1945)
vol. 102, p.223
S.Chandrasekhar

ON THE CONTINUOUS ABSORPTION COEFFICIENT OF THE NEGATIVE HYDROGEN ION

PCD STiAP Unit 0 Introduction to the course Select/Special Topics in Atomic Physics 42

We will also recognize that, the matrix elements for transitions can be obtained in different form like the length form, velocity form or what is called as momentum form. And there is also a form known as acceleration form and it was S. Chandrasekhar, who wrote to the formalism for this in a famous paper in 1945. So, we will acquaint ourselves with different alternative ways of the length form and the momentum form in particular of getting the matrix elements.

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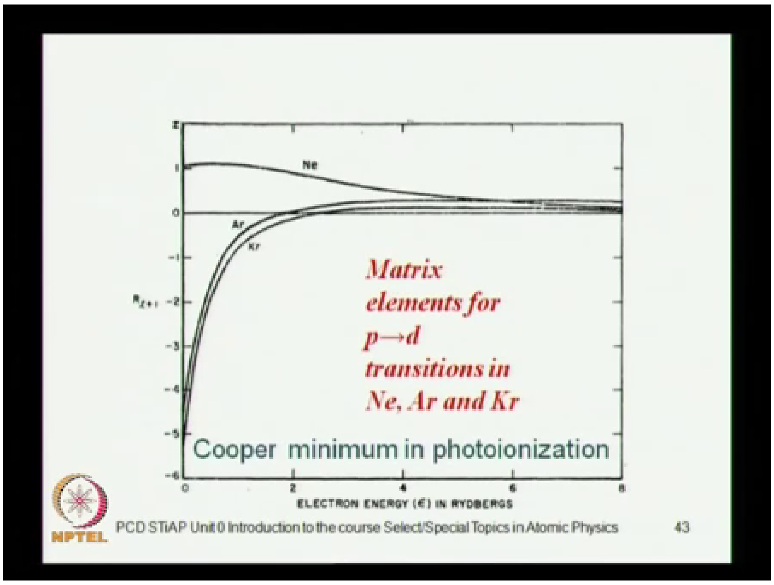

Matrix elements for p→d transitions in Ne, Ar and Kr

Cooper minimum in photoionization

PCD STiAP Unit 0 Introduction to the course Select/Special Topics in Atomic Physics

43

And we will find that, these matrix elements can actually undergo a transition in the sign, you can have matrix element, which is positive upto a certain energy and which changes that sign. For example, here for Argon you see that, this matrix element is negative, this is 0 and this is where, the matrix elements it is negative. And as energy increases from left to right, the matrix element changes, it undergoes change of sign over here and goes to 0.

And when it goes to 0, the matrix element vanishes, the corresponding probability vanishes and photo ionization cross section actually goes through a minimum, which is called as a Cooper minimum. And this is a property of gradients in photo ionization in physics, so you will get some introduction to this.

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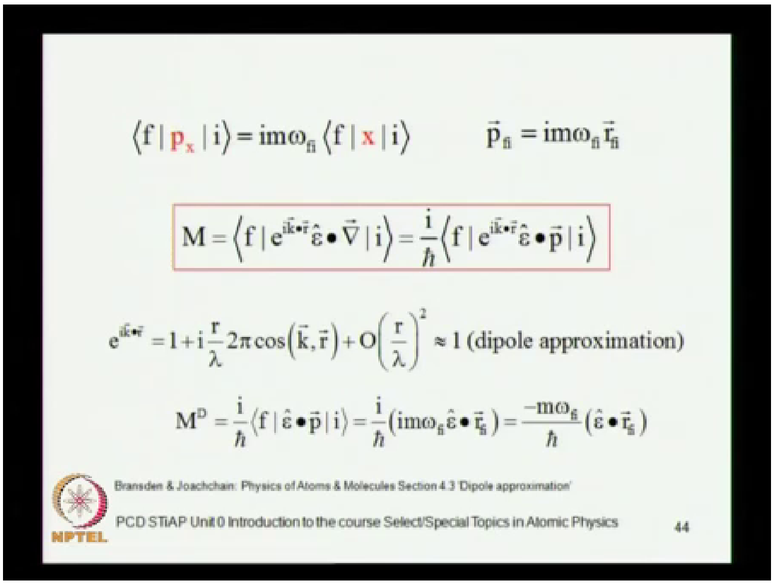

$$\langle f|p_x|i\rangle = im\omega_{fi}\langle f|x|i\rangle \qquad \vec{p}_{fi} = im\omega_{fi}\vec{r}_{fi}$$

$$\boxed{M = \left\langle f|e^{i\vec{k}\bullet\vec{r}}\hat{\varepsilon}\bullet\vec{\nabla}|i\right\rangle = \frac{i}{\hbar}\left\langle f|e^{i\vec{k}\bullet\vec{r}}\hat{\varepsilon}\bullet\vec{p}|i\right\rangle}$$

$$e^{i\vec{k}\bullet\vec{r}} = 1 + i\frac{r}{\lambda}2\pi\cos\left(\vec{k},\vec{r}\right) + O\left(\frac{r}{\lambda}\right)^2 \approx 1 \text{ (dipole approximation)}$$

$$M^D = \frac{i}{\hbar}\langle f|\hat{\varepsilon}\bullet\vec{p}|i\rangle = \frac{i}{\hbar}\left(im\omega_{fi}\hat{\varepsilon}\bullet\vec{r}_{fi}\right) = \frac{-m\omega_{fi}}{\hbar}\left(\hat{\varepsilon}\bullet\vec{r}_{fi}\right)$$

Bransden & Joachchain: Physics of Atoms & Molecules Section 4.3 'Dipole approximation'

You will also learn about, what is meant by a dipole approximation, what is the dipole approximation, why is call a dipole approximation and what are the consequence of dipole approximation. So, most of discussion will be essentially on the dipole approximation, but the toes that we will develop can be very easily extended to other multipole transition as well. And in modern way, atomic spectroscopy is certainly very necessary to go well beyond the dipole approximation, but you will get some sort of the start in that consideration.

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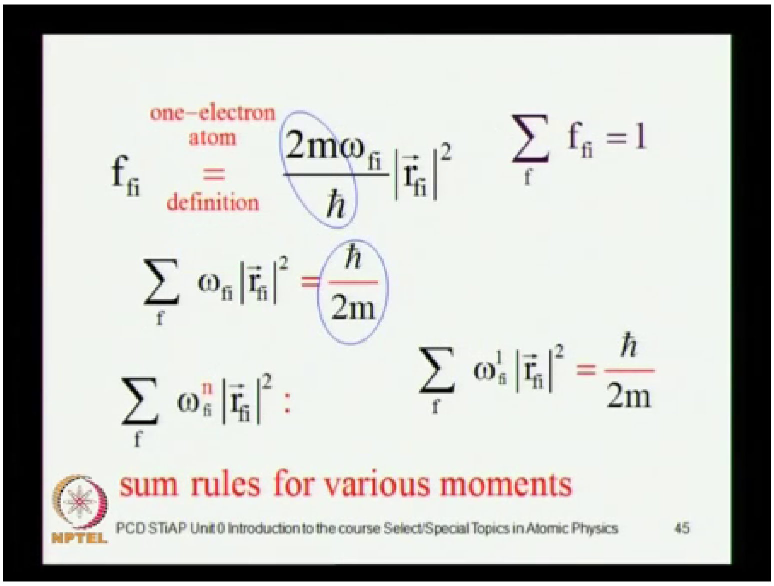

$$f_{fi} \overset{\text{one-electron atom}}{\underset{\text{definition}}{=}} \frac{2m\omega_{fi}}{\hbar}\left|\vec{r}_{fi}\right|^2 \qquad \sum_f f_{fi} = 1$$

$$\sum_f \omega_{fi}\left|\vec{r}_{fi}\right|^2 = \frac{\hbar}{2m}$$

$$\sum_f \omega_{fi}^n\left|\vec{r}_{fi}\right|^2 : \qquad \sum_f \omega_{fi}^1\left|\vec{r}_{fi}\right|^2 = \frac{\hbar}{2m}$$

sum rules for various moments

You will also learn about, what are known as sum rules, oscillators lying in sum rules like Thomas Riche Comb sum rules and so on. So, we will derive these expressions in this unit.

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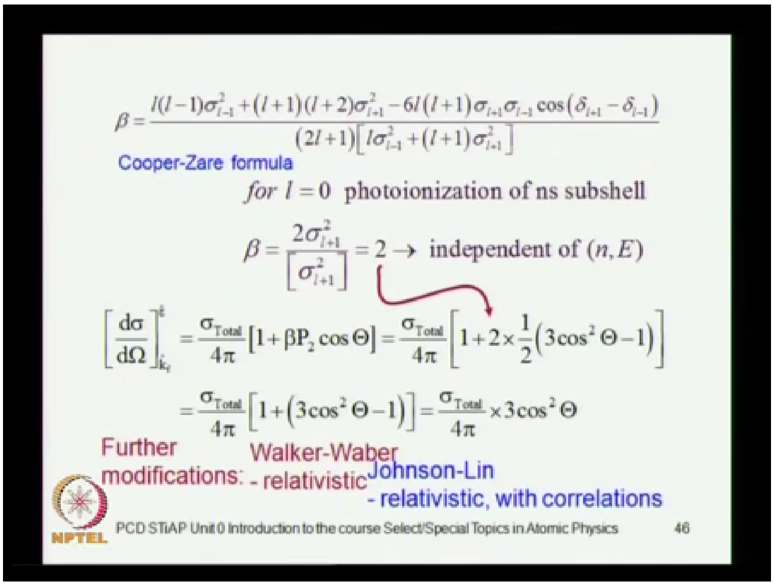

$$\beta = \frac{l(l-1)\sigma_{l-1}^2 + (l+1)(l+2)\sigma_{l+1}^2 - 6l(l+1)\sigma_{l+1}\sigma_{l-1}\cos(\delta_{l+1} - \delta_{l-1})}{(2l+1)\left[l\sigma_{l-1}^2 + (l+1)\sigma_{l+1}^2\right]}$$

Cooper-Zare formula

for $l = 0$ photoionization of ns subshell

$$\beta = \frac{2\sigma_{l+1}^2}{\left[\sigma_{l+1}^2\right]} = 2 \rightarrow \text{independent of } (n, E)$$

$$\left[\frac{d\sigma}{d\Omega}\right]_{\hat{k}_f}^{\hat{\varepsilon}} = \frac{\sigma_{\text{Total}}}{4\pi}\left[1 + \beta P_2 \cos\Theta\right] = \frac{\sigma_{\text{Total}}}{4\pi}\left[1 + 2 \times \frac{1}{2}\left(3\cos^2\Theta - 1\right)\right]$$

$$= \frac{\sigma_{\text{Total}}}{4\pi}\left[1 + \left(3\cos^2\Theta - 1\right)\right] = \frac{\sigma_{\text{Total}}}{4\pi} \times 3\cos^2\Theta$$

Further modifications: Walker-Waber - relativistic

Johnson-Lin - relativistic, with correlations

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And we will also get the famous Cooper Zare formula, which for angular distribution of photo electrons. So, they tell us, which is the direction, in which electrons are more likely to be emitted or if they are showing angular dependence, how is that angular dependence to be estimated. So, in the non relativistic quantum mechanics, this is done using a formalism developed by Cooper and Zare. So, you will learn the Cooper Zare formula, but of course, when you do relativistic quantum mechanics, you have to make corrections to the Cooper Zare formula.

So, the relativistic expressions what developed by Walker and Waber, and we will only give you the references for this, because it will go beyond the scope of this course. And then, you can also plug in the electron correlations, so you need a relativistic many body theory to get the correct expressions. And you will find it in the work by Johnson and Lin and some others also, so you will get some sort of interaction to the angular distribution of photo electrons.

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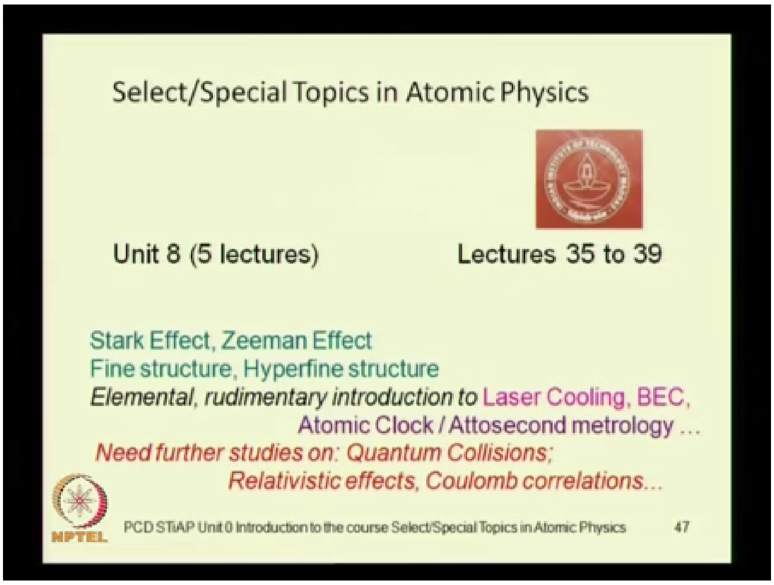

Select/Special Topics in Atomic Physics

Unit 8 (5 lectures) Lectures 35 to 39

Stark Effect, Zeeman Effect
Fine structure, Hyperfine structure
Elemental, rudimentary introduction to Laser Cooling, BEC,
Atomic Clock / Attosecond metrology ...
Need further studies on: Quantum Collisions;
Relativistic effects, Coulomb correlations...

And then, in the last unit, we will talk about an atom in various external fields, so we would have already consider interaction of an atom with electrometrical variation. So but in this unit, we will talk specifically about the famous Stark effect, the Zeeman effect, that we will also take into account further corrections like the fine structure, the hyperfine structure. And it will lead us to the consideration of somewhere exiting phenomena in modern day atomic physics when you also deal with quantum collisions, electron correlations and so on. Then, you get into the domain of exciting phenomena like laser cooling, Bose Einstein condensation, cooperative phenomena, correlated phenomena and fast processes, attosecond processes and so on, so this would be the subject.

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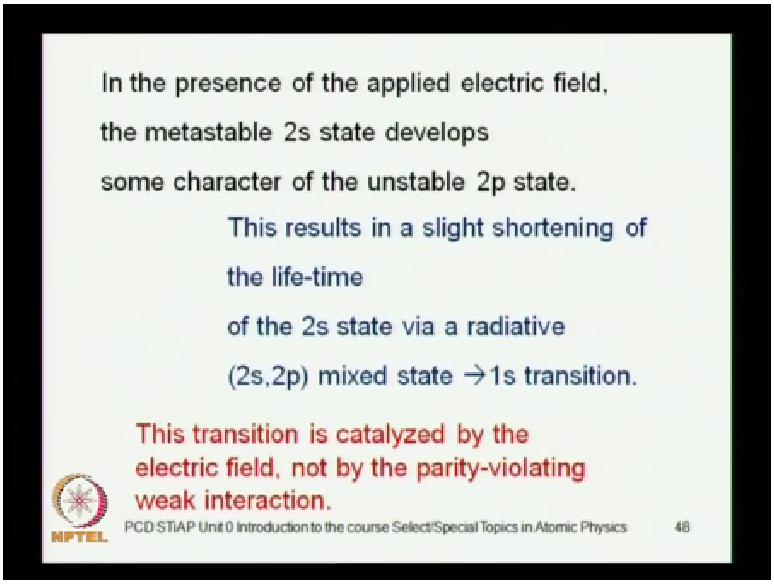

In the presence of the applied electric field, the metastable 2s state develops some character of the unstable 2p state.

This results in a slight shortening of the life-time of the 2s state via a radiative (2s,2p) mixed state →1s transition.

This transition is catalyzed by the electric field, not by the parity-violating weak interaction.

In unit 8, we will find that, in the presence of an external field, you have of the atom behaves differently, because the presence of the external field like the stark field for example, it can actually change the life time of an excited state. So, we will learn about some of these things when we deal with the Stark effect.

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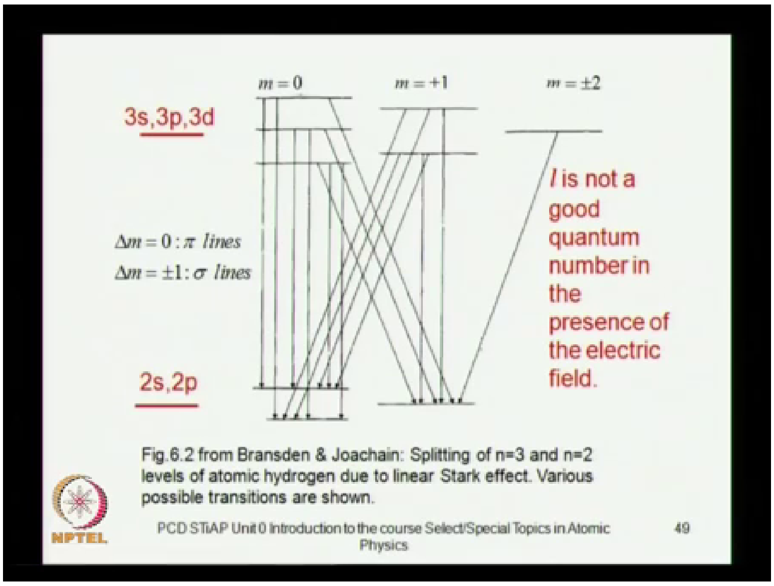

l is not a good quantum number in the presence of the electric field.

Fig.6.2 from Bransden & Joachain: Splitting of n=3 and n=2 levels of atomic hydrogen due to linear Stark effect. Various possible transitions are shown.

We will recognize that, in the presence of electric field, l is not a good quantum number, so you have to consider the transitions in the presence of an electric field. So, you have to use completely different kind of quantum mechanics, use perturbative methods dealing with degenerate states, so we will get some acquaintance with these techniques.

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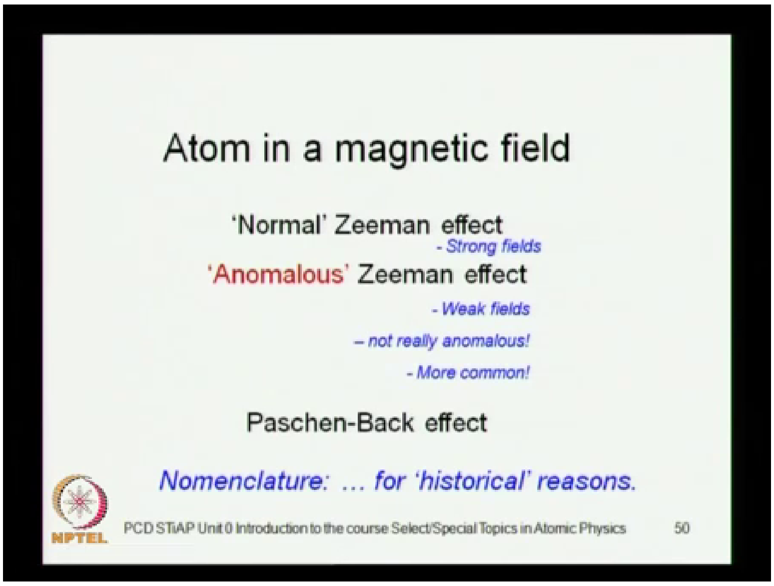

Atom in a magnetic field

'Normal' Zeeman effect

- Strong fields

'Anomalous' Zeeman effect

- Weak fields

– not really anomalous!

- More common!

Paschen-Back effect

Nomenclature: … for 'historical' reasons.

PCD STiAP Unit 0 Introduction to the course Select/Special Topics in Atomic Physics 50

And then, we will also learn about, what happens when you place atom in a magnetic field and there is a family of interactions, which are known as the Zeeman family. It includes, what is called the normal Zeeman effect, but also the anomalous Zeeman effect and also an effect, which is named after as Paschen and Back, and these are named differently just because they correspond to different magnitudes of the magnetic field that you can control.

But, for historical reasons, they have these different names and we will discuss, what is it that happens, how does an atom respond to a magnetic field. When you change the external magnetic field, you can make it strong or weak or moderate and these terms are qualitative terms. They obviously, have some implicit reference and the implicit reference in this consideration is the spin orbit interaction, which is internal to the atomic structure, so with reference to the spin orbit interaction, the field that you dealing with, which applying externally is a really weak or is it about the same value, equally strong or stronger. So, these are some of the considerations, that we will have in studying an atom in a magnetic field.

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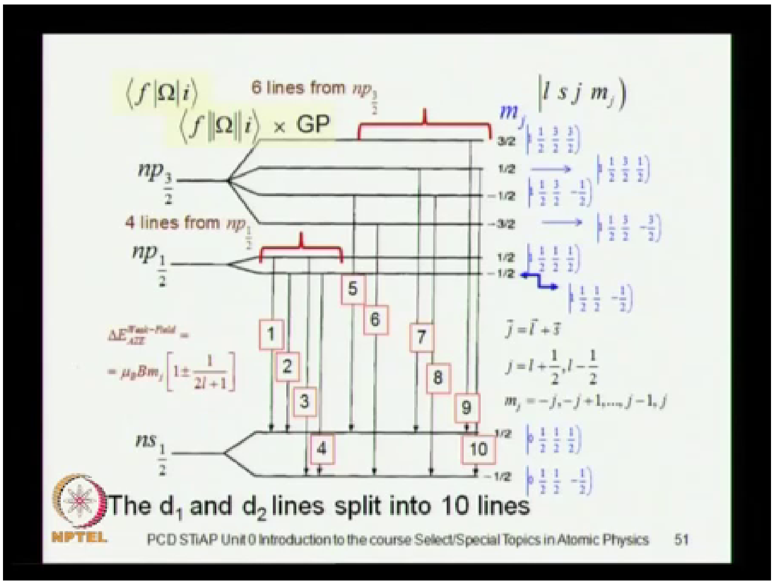

$$\Delta E^{Weak-Field}_{AZE} = \mu_B B m_j\left[1 \pm \frac{1}{2l+1}\right]$$

$$\vec{j} = \vec{l} + \vec{s}$$

$$j = l + \frac{1}{2}, l - \frac{1}{2}$$

$$m_j = -j, -j+1, \ldots, j-1, j$$

The d_1 and d_2 lines split into 10 lines

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We will find that, the D 1 D 2 lines gets split into large number of transition and you can study the spectroscopically.

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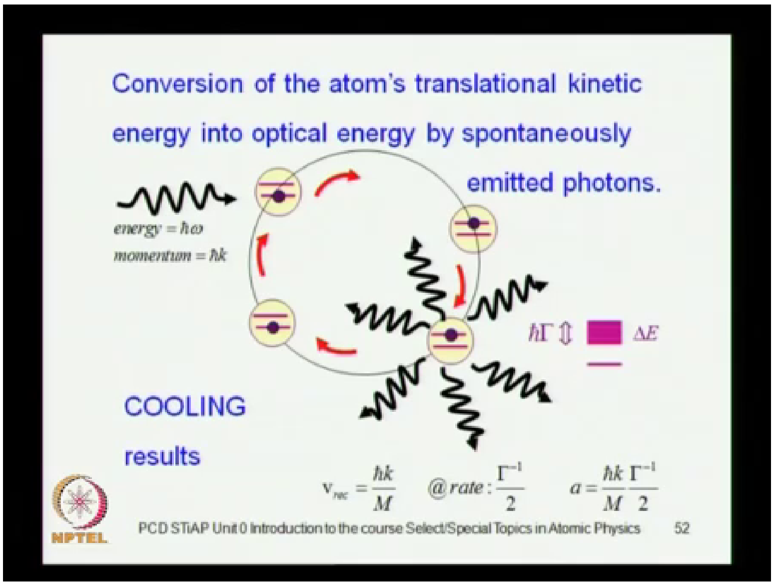

Conversion of the atom's translational kinetic energy into optical energy by spontaneously emitted photons.

$energy = \hbar\omega$

$momentum = \hbar k$

COOLING

results

$$v_{rec} = \frac{\hbar k}{M} \quad @rate: \frac{\Gamma^{-1}}{2} \quad a = \frac{\hbar k}{M}\frac{\Gamma^{-1}}{2}$$

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And then, we will also, once we have the tools for the Zeeman effect, we will also have studied the little bit of the hyperfine structure, how it effect energy level spectra, and how these can be exploited to subject and atom, to repeated cycles of cooling by exposing it to radiation pressure, the atom gets a cake. But then once it gets excited as a result of absorption of this electronic energy when it comes down to the ground states, it emits the absorbed energy in random directions. And when this is done cyclically, the atom would actually cool down, so this is the essence of laser cooling and we will discuss some of this towards the end of the unit 8.

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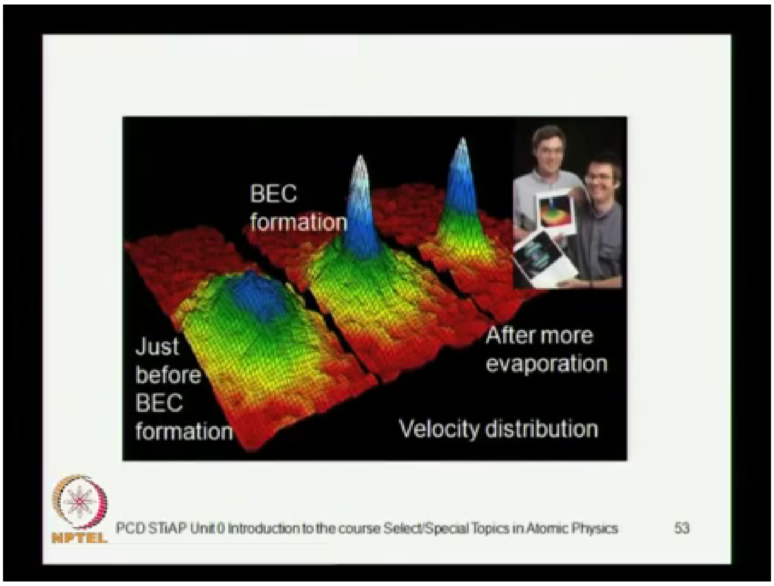

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In fact, when the momentum of the atom comes down, this de Broglie wavelength increases, lambda is h over p, so lambda increases. And if the atoms are bosons, you can actually get Bose Einstein condensation, so we will introduce you to this.

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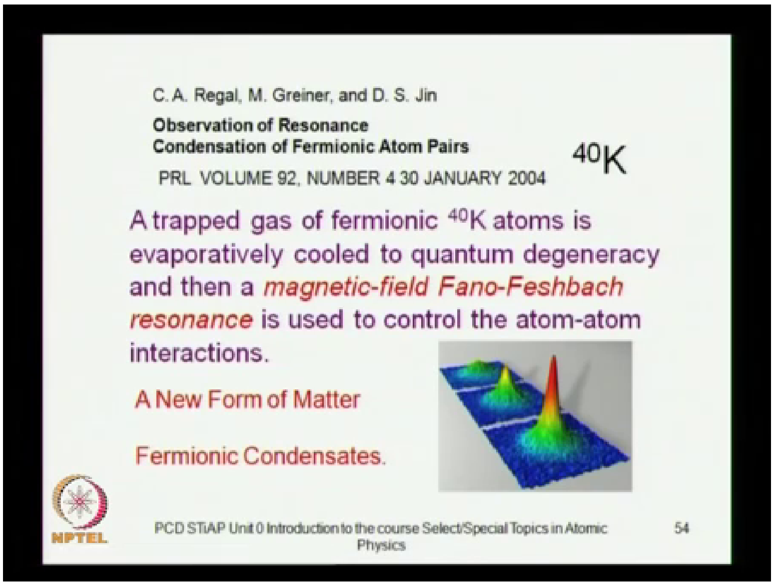

C. A. Regal, M. Greiner, and D. S. Jin

Observation of Resonance Condensation of Fermionic Atom Pairs

PRL VOLUME 92, NUMBER 4 30 JANUARY 2004

^{40}K

A trapped gas of fermionic ^{40}K atoms is evaporatively cooled to quantum degeneracy and then a *magnetic-field Fano-Feshbach resonance* is used to control the atom-atom interactions.

A New Form of Matter

Fermionic Condensates.

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We will also talk about Fermi mixtures, because you can have Fermion atoms, which can constitute pears and you can pear them using some external controls like magnetic fields, which will induce certain resonant phenomenon by controlling the scattering line. So, that requires tools in quantum collision theory and in particular, the things like that Fano Feshbach resonance is exploited this, so that you can form completely new states of matter like the Fermionic condensates.

So, the Bose Einstein condensates itself is a different kind of matter, which perhaps does not exist anywhere else in the universe, may be it does. If there is life elsewhere and they did it before they ask, I have no idea about that. But then, it is the different kind of state of matter all together and then, you can also have the Fermionic condensates.

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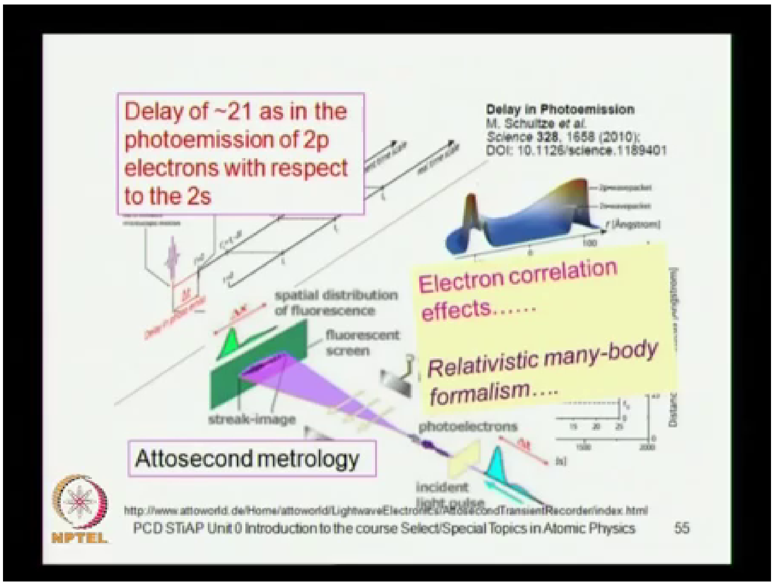

Delay of ~21 as in the photoemission of 2p electrons with respect to the 2s

Delay in Photoemission
M. Schultze *et al.*
Science **328**, 1658 (2010);
DOI: 10.1126/science.1189401

Electron correlation effects……

Relativistic many-body formalism….

Attosecond metrology

http://www.attoworld.de/Home/attoworld/LightwaveElectronics/AttosecondTransientRecorder/index.html

So, this enables us to develop cool down the atoms, which is the good think to measure time, because you need slow atoms and cooled atoms to measure time accurately. And you need extremely high accuracy in the measurement of time at the logal of attoseconds and that is the current day technology that people are developing. But, to study this, one requires fairly sophisticated tools in quantum collisions theory is well as in the study of many electron systems.

And in particular, the coulomb correlations, which we had sort of averaged out in the Hartree Fock formalism, which we would have leveled out or averaged out at the Hartree Fock level or in the Dirac Hartree Fock. These correlations effects are not taken into account and they must be taken into account to study this phenomena. So, that becomes a subject of a different course and this is pretty much the overview of this course.

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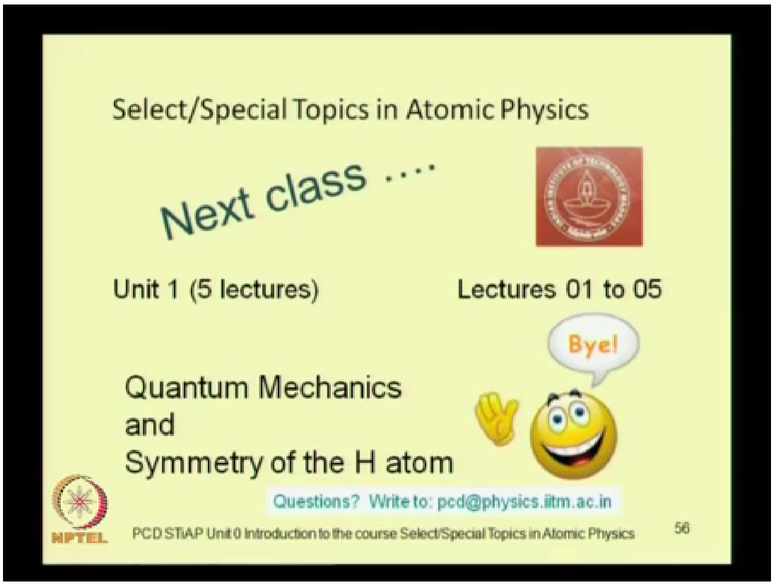

Select/Special Topics in Atomic Physics

Next class ....

Unit 1 (5 lectures)

Lectures 01 to 05

Quantum Mechanics
and
Symmetry of the H atom

Questions? Write to: pcd@physics.iitm.ac.in

And in the next class, we will begin with the quantum mechanics of the hydrogen atom, so any questions can certainly be sent to me.

Thank you.