

Select/Special Topics in
'Theory of Atomic Collisions and Spectroscopy'
Prof. P.C. Deshmukh
Department of Physics
Indian Institute of Technology-Madras

Lecture 01
Introductory Lecture - Course Overview

(Refer Slide Time: 00:27)



Greetings, welcome to this course on theory of atomic collisions and spectroscopy. So, I will make an attempt to provide you with an overview of what to expect in this course and I would like to remind you of something that we would have referred to in one of our earlier courses in atomic physics which is a quote from a very distinguished physicist who ventured to speculate on what would one leave behind for posterity.

(Refer Slide Time: 01:03)

*"If, in some cataclysm, all 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? **I believe it is the atomic hypothesis (or atomic fact, or whatever you wish to call it) that all things are made of atoms -**"*

"... in that one sentence you will see an enormous amount of information about the world, if just a little imagination and thinking are applied."

**The Feynman Lectures on Physics,
Vol 1, Sec 1-2,
Science in one line for posterity....**

3



If you could write and describe science and only one line if everything else were to perish, now this almost sounds like a very arrogant attempt as to how could one thing that you can even attempt to do that. But the person who did it was fully qualified to make such an attempt it was none other than Richard Feynman and this is a quote from Feynman lectures and what he says in this is that.

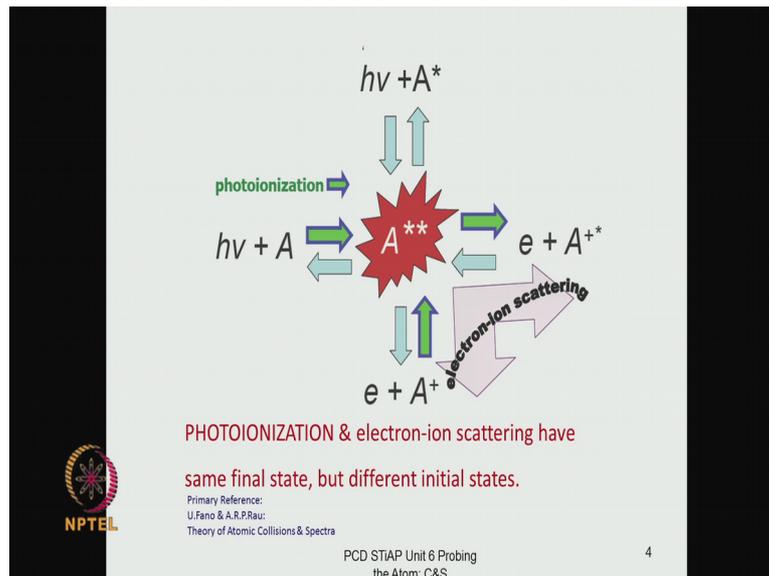
If in some Cataclysm all scientific knowledge were to be destroyed and only one sentence passed on to the next generation of creatures, what statement would contain the most information in the fewest words. Now Feynman goes on to answer this and he says that it is the atomic hypothesis that all things are made of atoms now that is his answer.

And he goes on to clarify that in that one sentence you will see an enormous amount of information about the world if just a little imagination but of course it is not the imagination of an ordinary man it is the imagination of someone like Feynman if you add a little bit of imagination then you know one could extract a lot of science.

Now it is very fascinating to you know speculate on this question why would Feynman choose this particular atomic hypothesis to be the one line in which he could transfer the most information for posterity. And I really do not know what Feynman's reasons were but if we if we sit together and apply our minds then I think one could guess that okay by studying the physics of atoms one could really get a lot of information.

And it does require a little bit of imagination as Feynman say is very neatly in this quote but you could extract quantum mechanics, you could extract relativity out of it, you could extract quantum statistics out of it and so much of the fundamentals of science could come out of atomic physics. Which is what makes this subject so fascinating, so complete and so important.

(Refer Slide Time: 03:40)



So, having said that I would think that okay it is very important to study atomic physics in one's graduate studies in physics and one could study it in a variety of ways because you have an atom and then you can use certain kinds of probes. And you can either use electromagnetic radiation which is here so $h\nu$ is a photon and if A is a neutral atom.

Then you could have a photon atom interaction to probe the atom and see what kind of results you would get or you could also target this using an electron and you can do scattering. This is what typically one would call a scattering and these details I have dealt with in different at a different point of this course and one of the previous courses as well.

So, I am not getting into those details but the point that I want to highlight over here that photon matter interaction and quantum collisions are the two fundamental probes, to probe an atomic system. And the atomic system is then the fundamental thing which is of most importance if we go by Feynman's code.

And this kind of interaction makes the subject of collisions and spectroscopy extremely important. These two processes collisions and spectroscopy when you are probing with electromagnetic radiation you do spectroscopy and these two processes are in fact related to each other through time reversal symmetry. So, I think these are issues of details which I will not get into in this introductory class.

(Refer Slide Time: 05:26)

Who is this course for?
This course is for those students who have taken first courses in quantum mechanics / atomic physics.

Sequel to:
 Select/Special Topics in Atomic Physics
 Quantum Mechanics
<http://nptel.iitm.ac.in/courses/115106057/>

How would you benefit most from this course?

- Download the PDF files from the course website.
- Refer to the PDF files before, during and after the lectures.
- You may open these PDF files in another window while listening to the lecture in a small window on your screen.



PCD TACS Unit 1 Select/Special Topics from 'Theory of Atomic Collisions & Spectroscopy'

So, let me give you a general overview of this course and first of all I would like to tell you who this course is for and this course is developed as a sequel to another course which I offered for the NPTEL which is on select or special topics in atomic physics. And as such this course can also be considered as the select topics in quantum mechanics.

And this is not surprising because quantum mechanics and atomic physics grew hand in hand in the 20th century. So, all developments in atomic physics and all developments in quantum mechanics went progressed together in the early days of quantum theory.

Which is why an introductory course in atomic physics strongly overlaps with an introductory course in quantum mechanics, so anybody who has taken an introductory course in quantum mechanics or atomic physics is well suited to take this course which we are described, which we are introducing in today's class which is on select or special topics in the theory of atomic collisions and spectroscopy.

Now I would like to point out how to benefit most from this course because I have used PowerPoint slides to discuss various materials. It takes good amount of time to prepare those slides but the advantage is that the corresponding PDF files can be prepared and these are uploaded at the course website.

So, you can download these PDF files and that is the first recommendation I will like to make that download these PDF files from the course website and you can use these PDF files before viewing the video lecture, during the time that you are viewing the lecture or after it, because then all of that material is available.

(Refer Slide Time: 07:30)

Select/Special Topics from 'Theory of Atomic Collisions and Spectroscopy'
46 Lectures

Unit No.	Topic	Lectures
1	Introduction to the course	This lecture, 01
	Quantum Theory of Collisions – Part 1	02 to 12
2	Quantum Many-body theory, Electron correlations, Second Quantization	13 to 15
3	Electron Gas in the Hartree-Fock and the Random Phase Approximation	16 to 24
4	Feynman Diagram Methods	25 to 32
5	Quantum Theory of Collisions – Part 2 Lippman-Schwinger Equation, Born Approximations, Coulomb Scattering	33 to 35
6	Quantum Theory of Collisions – Part 3 Resonances in Quantum Collisions, phase shifts, resonance widths, time-delay	36 to 39
7	Quantum Theory of Collisions – Part 4 Fano-Feshbach and Shape Resonances; Life-times and time-delay in scattering	40 to 43
8	Three Guest Lectures by Prof.S.T.Manson (GSU, Atlanta)	44 to 46

NPTEL

PCD TACS Unit 1 Select/Special Topics from 'Theory of Atomic Collisions & Spectroscopy' 7

The other advantage is that you do not have to take notes while going listening to the lecture because all the PDF files have got the complete description of the topic and you will have them handy already. So, you can just pay attention on the discussion itself and go through the lectures. So, this course is, there will be 46 lectures in this course including this lecture which is the introductory lecture.

And then we will have a number of units in the first unit I will introduce quantum theory of collisions this will be a second part of what we did in the earlier course in atomic physics. So, some background will be assumed about collision physics. In the second unit we will do quantum many-body theory, discuss second quantization methods so that we can address the subject of electron correlations in many electron systems.

In the third unit we will go beyond the Hartree Fock method because the Hartree Fock which gives you an excellent starting point but then for detailed calculations and detailed analysis of atomic structure and dynamics you need to take into account electron correlations which are excluded in the Hartree Fock formalism. And to be able to do that there are a number of ways of doing it one of the very powerful ways of doing it is the linearization technique.

And this can be done using a variety of ways. One of the formalism is due to Bohm and Pines which is known as a Random Phase Approximation and this name applies to other methods of linearization techniques in this particular context. So we will discuss the Bohm Pines method in unit 3. Then we will also introduce Feynman diagrammatic methods and get into the ring diagrams which correspond to the linearization technique which is also used in Bohm and Pines.

Then we will get back to quantum collisions and do a few problems which are of major importance like the Lippman Schwinger equation, the Born approximation. We will also do the Coulomb Scattering and we will then deal with resonances in quantum collisions. And then we will do a Fano analysis using the final shape parameters of the Fano Fechbach resonances.

We will deal with lifetimes and time delays in scattering and also in the photoemission process. Then we have one unit in which we will have some guest lectures by my long time research collaborator professor S.T. Manson, he has given three lectures which will be appended to this course toward the end.

In which he will show some applications of you know the techniques which have been introduced in this course. So, these this is the general overview of the course. So, now let me give you one specific information that the unit 2, 3 and 4 which is on quantum many-body theory and many electron methods.

So these three units can be done even toward the end of the course, so not necessarily after unit one. So, if you want you can jump from unit 1 to unit 5 and so on okay. When the whole course is ready you could do that but you can do it in any sequence. So, these three form one sort of group and then the other units which have in which I deal with quantum theory of collisions part 1, part 2, part 3 and part 4. They can also be done together in one go.
(Refer Slide Time: 11:03)

Select/Special Topics in Atomic Physics

Unit 1 (This, + 11 lectures)

Lectures 02 to 12
Quantum Theory of Collisions – Part 1.

PCD TACS Unit 1 Select/Special Topics from 'Theory of Atomic Collisions & Spectroscopy' 8

So, in part 1 of the quantum collision theory;
(Refer Slide Time: 11:07)

Incident beam of Monoenergetic particles

Detector

Target

$A + B \rightarrow A + B$ (elastic scattering)

$A + B \rightarrow A^* + B$ (inelastic scattering)

$A + B \rightarrow A^* + B^*$ * denotes new internal state

$A + B \rightarrow C + D$ ← reactive scattering - rearrangement when colliding particles are composite objects.

“channel” : possible mode of fragmentation pathway

PCD TACS Unit 1 Select/Special Topics from 'Theory of Atomic Collisions & Spectroscopy'

9

I will basically describe the collision process deal with different kinds of collisions inelastic collisions. Then we will even talk about reactive scattering, inelastic collisions, elastic collisions and so on. And then we will discuss what our collision pathways? What are different collision channels?
(Refer Slide Time: 11:29)

cross-section =

$$= \frac{\text{number of events per unit time per unit scatterer}}{\text{flux of the incident particles w.r.t. the target}}$$

$$\uparrow \sigma_{tot} = \frac{P \times N_A}{\Phi_A n_B} \uparrow$$

Scattering cross section

direction of incident beam

effective target area that interacts with the incident beam and scatters it

“tendency” of particles A & B to interact

PCD TACS Unit 1 Select/Special Topics from 'Theory of Atomic Collisions & Spectroscopy'

9

So we will introduce the vocabulary of doing collision physics we will define the cross section carefully as the number of events per unit time per unit scatter. It is the ratio of this to the flux of incident particles with respect to the target. So, starting with the fundamentals of what exactly is a scattering cross section. We will develop the formalism;
(Refer Slide Time: 11:51)

Θ : operator for
TIME REVERSAL SYMMETRY

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

collision = photoionization

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

Please refer to details from:
PCD STAP Unit 6 Probing the Atom
Lecture link: <http://nptel.iitm.ac.in/courses/115106057/27 & /28 & /29 & /30>
PCD TACS Unit 1 Select/Special Topics from 'Theory of Atomic Collisions & Spectroscopy'

11

We will refer to this relationship between collisions and photo ionization. Which is through time reversal symmetry we have done this somewhat extensively in the previous course which is also an NPTEL course which is a special topics in atomic physics and this was done in unit 6 of that but we will use some of these results in this course as well. So, we will make use of the relationships between the solutions to the quantum problem for collisions and for photo ionization.

(Refer Slide Time: 12:23)

$C_l = e^{i\delta_l(k)}$ Outgoing wave boundary condition

'collisions'

$$\psi_{\vec{k}_i}^{\oplus}(\vec{r}; r \rightarrow \infty) \rightarrow A(k) \left[e^{i\vec{k}_i \cdot \vec{r}} + \frac{f(\hat{\Omega})}{r} e^{ikr} \right]$$

$$f(k, \theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) [e^{2i\delta_l(k)} - 1] P_l(\cos \theta)$$

Contributions of Faxen-Holtmark's formalism
the partial waves to the scattering amplitude.

Reference: **Quantum Theory of Collisions** by Charles J Joachain
North-Holland Publishing Co. // Section 3.2 // see Eq.3.27, page 49

12

Via the time reversal symmetry and then do formal collision physics without going away boundary conditions so, we will develop the Faxen Holtzmark's mark equation for the scattering amplitude and so on.

(Refer Slide Time: 12:40)



$$\iint [f(\hat{n}, \hat{n}') - f^*(\hat{n}', \hat{n})] F(\hat{n}) dO =$$

$$= \frac{ki}{2\pi} \left[\iint f^*(\hat{n}', \hat{n}'') \iint f(\hat{n}, \hat{n}'') F(\hat{n}) dO dO'' \right]$$

$$\iint [f(\hat{n}, \hat{n}') - f^*(\hat{n}', \hat{n})] F(\hat{n}) dO =$$

$$= \iint \left\{ \frac{ki}{2\pi} \iint f^*(\hat{n}', \hat{n}'') f(\hat{n}, \hat{n}'') dO'' \right\} F(\hat{n}) dO$$

for $\hat{n}' = \hat{n}$

$$f(\hat{n}, \hat{n}') - f^*(\hat{n}', \hat{n}) = \frac{ki}{2\pi} \iint f^*(\hat{n}', \hat{n}'') f(\hat{n}, \hat{n}'') dO''$$

$$f(\hat{n}, \hat{n}) - f^*(\hat{n}, \hat{n}) = \frac{ki}{2\pi} \iint f^*(\hat{n}, \hat{n}'') f(\hat{n}, \hat{n}'') dO'' \quad \hat{S}: \text{unitary}$$

$$2i \operatorname{Im} [f(\hat{n}, \hat{n})] = \frac{ki}{2\pi} \iint |f(\hat{n}, \hat{n}'')|^2 dO'' \quad |f(\hat{n}, \hat{n}'')|^2 = \frac{d\sigma}{dO''}$$

$$2i \operatorname{Im} [f(\hat{n}, \hat{n})] = \frac{ki}{2\pi} \sigma_{\text{Total}} \quad \sigma_{\text{Total}} = \frac{4\pi}{k} \operatorname{Im} [f(\hat{n}, \hat{n})] \quad \text{optical theorem}$$

PCD TACS Unit 1 Select/Special Topics from 'Theory of Atomic Collisions & Spectroscopy'

13

So, we will introduce all of these parameters or phase shifts. We will do the optical theorem; we will discuss the unitarity of the S operator, the sketching operator. And as you see from these slides there are a number of mathematical equations and it would take you some time to take notes which you do not have to.

Because all of this is available in the PDF file which is why I said at the very outset that a good idea to take this course is to download those PDF files at the very beginning and keep them handy you can even have them in one window and listen to the video lecture in another window.

(Refer Slide Time: 13:14)



interchange incidence & scattered directions
& reverse signs $S(\hat{n}, \hat{n}') = S(-\hat{n}', -\hat{n})$

scattering amplitudes: $f(\hat{n}, \hat{n}') = f(-\hat{n}', -\hat{n})$

RECIPROCITY THEOREM

The scattering amplitudes for two scattering processes which are time-reversed processes of each other are the same.

PCD TACS Unit 1 Select/Special Topics from 'Theory of Atomic Collisions & Spectroscopy'

14

We will also do what is known as the reciprocity theorem. This also reflects on the time reversal symmetry. So, all this will be done in unit 1.

(Refer Slide Time: 13:21)

Partial wave analysis

Low energy ($\sim 1\text{eV}$) scattering of electrons by rare gas atoms – Xe, Kr, Ar

$$\sigma_{\text{Total}} = \sum_{l=0}^{\infty} \sigma_l(k)$$

$$\sigma_l(k) = \frac{4\pi}{k^2} (2l+1) \sin^2 [\delta_l(k)]$$

$l_{\text{max}} \sim ka$ Consider s-wave scattering

$\delta_{l=0}(k) \rightarrow n\pi$ Ramsauer-Townsend effect

Electrons just go through the target! – no scattering!

Fig. 4. The probability of scattering P_s as a function of $(V - V_0)^{1/2}$, where $V - V_0$ is the electron energy. Ionization occurs at $(V_0)^{1/2}$.

Demonstration of Ramsauer Townsend Effect in Xenon by Kukolich – Am. J. Phys. 1968 Vol.36, No.8, p701-703

PCD TACS Unit 1 Select/Special Topics from Theory of Atomic Collisions & Spectroscopy 15

We will deal with some special cases in which you have a target, you have an incident beam of projectiles but if you look at the scattered flux it would appear under certain conditions as if there was no scattering at all. As if the scattering has disappeared as if the target has vanished. And this is what is referred to as the Ramsauer Townsend Effect as to why you have this effect. So, we will look into some detailed aspects of this. (Refer Slide Time: 14:09)

How the s-wave phase shift changes with the strength of the potential

$\delta_0(k \rightarrow 0) = n_0\pi$

$n_0 = \text{number of bound states}$

Levinson's theorem

$\frac{\pi}{2} \approx 1.57 \uparrow$

$\frac{3\pi}{2} \approx 4.71 \uparrow$

$\frac{5\pi}{2} \approx 7.85 \uparrow$

π

2π

3π

βa

PCD TACS Unit 1 Select/Special Topics from Theory of Atomic Collisions & Spectroscopy 16

This has closed bearing on also related theorem which is known as the Levinson theorem which we will discuss and it will deal with what is the scattering phase shift at the threshold and how it is related to the number of bound states of an attractive potential because it will have a certain finite number of bound states so that is the question we will address in this. (Refer Slide Time: 14:18)

"EFFECTIVE RANGE"

$U(r)$ vs r graph showing a square well of depth $-\beta^2$ for $r < a$ and zero for $r > a$.

$U(r) = \frac{2m}{\hbar^2} V(r)$ for $r < a$

$U(r) = -\beta^2$ for $r < a$

$U(r) = 0$ for $r > a$

$\frac{2mE}{\hbar^2} = k^2 > 0$

$u_{e,l}(r) = rR_{e,l}(r)$

PHYSICAL REVIEW VOLUME 76, NUMBER 1 JULY 1, 1949

Theory of the Effective Range in Nuclear Scattering

H. A. BETHE
Physics Department, Cornell University, Ithaca, New York*

Neutron-Proton scattering
→ Spin dependent

Theory of ultracold atomic Fermi gases
REVIEWS OF MODERN PHYSICS, VOLUME 80, OCTOBER-DECEMBER 2008
Stefano Giorgini *et al.*

PCD TACS Unit 1 Select/Special Topics from Theory of Atomic Collisions & Spectroscopy / 17

And we will also introduce the effective range theory which was developed by Bethe. It will have some applications and some problems of current interest. In which you will find this to have interesting applications is on cold atoms and Bose Einstein condensation including the condensation of Fermi mixtures.
(Refer Slide Time: 14:38)

Energy vs Interatomic distance graph showing a bound state and a scattering length α .

FANO FESHBACK RESONANCE

scattering length α

Free, unbound state of the two Fermionic atoms

$\alpha < 0$

"open channel" $S=1$ BCS

"closed" $S=0$ BEC

In between, scattering length diverges

Molecular, bound state of the two Fermionic atoms

Ultracold, low energy s-wave scattering of two Fermionic atoms

PCD TACS Unit 1 Select/Special Topics from Theory of Atomic Collisions & Spectroscopy / 18

In which you use these techniques and discuss this transformation from a BCE to a BCS state and so on. So some of these are done via and exploiting the physics of the Fano Feshbach Resonances so some of these things will be introduced in this unit.
(Refer Slide Time: 14:58)

Select/Special Topics from
'Theory of Atomic Collisions and Spectroscopy'



Unit 2 (3 lectures) Lectures 13 to 15

Quantum Many-body theory, Electron correlations, Second Quantization



PCD TACS Unit 1 Select/Special Topics from 'Theory of Atomic Collisions & Spectroscopy' 19

Then we get into the formalism of many electron theories and in particular we will introduce the second quantization method which is a very powerful language to deal with the many electron problems. And it gives you a very nice handle on developing techniques which go beyond the Hartree Fock.

So, the Hartree Fock remains within the domain of the single particle approximation although of course it does deal with the N electron system. But it deals only with the anti-symmetric nature so it takes into account the Fermi Dirac statistics, the Fermi Dirac correlations but not the Coulomb correlation. So, those are the ones which methods of second quantization will help us address.

(Refer Slide Time: 15:43)

$Z = 12$

Slater determinant $\psi_1^{SD} = 1s_1^2 2s_1^2 2p_1^2 2p_3^4 3s_1^2$

$\psi_2^{SD} = 1s_1^2 2s_1^2 2p_1^2 2p_3^4 3p_1^2$

..... Many different Slater determinants can be used!

Multi-configuration Hartree-Fock:
CI: Configuration Interaction *Many-Body Correlations*



PCD TACS Unit 1 Select/Special Topics from 'Theory of Atomic Collisions & Spectroscopy' 20

So, we will take up some examples of what a configuration interaction will do so that a single Slater determinant of the Hartree Fock will not be a sufficient description of the N electrons

state. You need multi configurational Hartree Fock or multi configuration Dirac Hartree Fock, if you were to be using relativistic wave functions.
(Refer Slide Time: 16:19)

Fermion (electron) creation and destruction operators

Properties $|\Psi(t)\rangle = \sum_{n_1=0}^1 \dots \sum_{n_i=0}^1 \dots \sum_{n_s=0}^1 f(n_1, \dots, n_i, \dots, n_s, t) |n_1, n_2, \dots, n_s\rangle$

fundamental anti-commutation rules

for fermion operators:

$$[a_r, a_s^\dagger]_+ = \delta_{rs} \quad [a_r^\dagger, a_s^\dagger]_+ = 0 \quad [a_r, a_s]_+ = 0$$

fundamental commutation rules

for boson operators: *commutator: [A, B] = AB - BA*

$$[b_r, b_s^\dagger]_- = \delta_{rs} \quad [b_r^\dagger, b_s^\dagger]_- = 0 \quad [b_r, b_s]_- = 0$$

PCD TACS Unit 1 Select/Special Topics from 'Theory of Atomic Collisions & Spectroscopy' 21

And the second quantization methods give you a very nice handle on addressing such configuration interactions which are involved in electron correlations. So, the second quantization methods, you know the fundamental quantities for these are the Fermion and Boson electron creation and destruction operators. So, the whole formalism is developed in terms of the second quantization operators.
(Refer Slide Time: 16:33)

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \left[\sum_r \sum_s a_r^\dagger a_s \langle r|T|s\rangle + \frac{1}{2} \sum_r \sum_s \sum_t \sum_u a_r^\dagger a_s a_t^\dagger a_u \langle rs|V|tu\rangle \right] |\Psi(t)\rangle$$

$$H = \sum_r \sum_s a_r^\dagger a_s \langle r|T|s\rangle + \frac{1}{2} \sum_r \sum_s \sum_t \sum_u a_r^\dagger a_s a_t^\dagger a_u \langle rs|V|tu\rangle$$

$$a_r^\dagger a_t a_s^\dagger a_u = -a_r^\dagger a_s^\dagger a_t a_u = a_r^\dagger a_s^\dagger a_u a_t$$

$$H = \sum_r \sum_s a_r^\dagger a_s \langle r|T|s\rangle + \frac{1}{2} \sum_r \sum_s \sum_t \sum_u a_r^\dagger a_s a_t^\dagger a_u \langle rs|V|tu\rangle$$

$$H = \sum_r \sum_s a_r^\dagger \langle r|T|s\rangle a_s + \frac{1}{2} \sum_r \sum_s \sum_t \sum_u a_r^\dagger a_s^\dagger \langle rs|V|tu\rangle a_u a_t$$

...Eq.1.60 / F & W / p.18 Note: †Order†

$$\langle rs|V|tu\rangle = \int dq_1 \int dq_2 \phi_r^*(q_1) \phi_s^*(q_2) V(q_1, q_2) \phi_t(q_1) \phi_u(q_2)$$

PCD TACS Unit 1 Select/Special Topics from 'Theory of Atomic Collisions & Spectroscopy' 22

And we will develop a handle on this. We will write the many electrons Hamiltonian in terms of the second quantization operators.
(Refer Slide Time: 16:42)

Select/Special Topics in Atomic Physics



Unit 3 (10 lectures) Lectures 16 to 25

Electron Gas in the Hartree-Fock and
the Random Phase Approximation



PCD TACS Unit 1 Select/Special Topics from 'Theory of Atomic Collisions & Spectroscopy'

23

And then I will get into the details of the Random Phase Approximation which is to go beyond the Hartree Fock. And then we will take the classic example of the electron gas in the random phase approximation. So, the Hartree Fock we have already done in the previous course and we will now consider the electron gas in the random phase approximation. (Refer Slide Time: 17:07)

Complete expressions for the Hamiltonian, inclusive of spin labels

$$[c_{\alpha\sigma_1}, c_{\alpha\sigma_2}]_{\pm} = \delta_{\alpha\sigma_1} \delta_{\sigma_1\sigma_2} \quad [c_{\alpha\sigma_1}, c_{\alpha\sigma_2}]_{\pm} = 0 \quad [c_{\alpha\sigma_1}, c_{\alpha\sigma_2}]_{\pm} = 0$$

$$H = \int \hat{\psi}_{\alpha}^{\dagger}(q) f(q) \hat{\psi}_{\beta}(q) dq + \frac{1}{2} \int \int \hat{\psi}_{\alpha}^{\dagger}(q) \hat{\psi}_{\beta}^{\dagger}(q) v(q, q') \hat{\psi}_{\gamma}(q') \hat{\psi}_{\delta}(q) dq dq'$$

$$\hat{\psi}_{\alpha}(q) = \sum_{\alpha} \sum_i \psi_{i\alpha}(q) c_{i\alpha} \quad \hat{\psi}_{\beta}^{\dagger}(q) = \sum_{\beta} \sum_j \psi_{j\beta}^{*}(q) c_{j\beta}^{\dagger}$$

$$H = \sum_{\alpha} \sum_{\beta} c_{\alpha}^{\dagger} \int \psi_{i\alpha}^{*}(q) f(q) \psi_{j\beta}(q) dq c_{\beta} +$$

$$+ \frac{1}{2} \sum_{\alpha} \sum_{\beta} \sum_{\gamma} \sum_{\delta} c_{\alpha}^{\dagger} c_{\beta}^{\dagger} \int \int \psi_{i\alpha}^{*}(q) \psi_{j\beta}^{*}(q) v(q, q') \psi_{\gamma}(q') \psi_{\delta}(q) dq dq' c_{\gamma} c_{\delta}$$

$$H = \sum_{\alpha} \sum_{\beta} c_{\alpha}^{\dagger} \langle i\alpha | f | j\beta \rangle c_{\beta} + \frac{1}{2} \sum_{\alpha} \sum_{\beta} \sum_{\gamma} \sum_{\delta} c_{\alpha}^{\dagger} c_{\beta}^{\dagger} \langle i\alpha, j\beta | v | l\delta, k\gamma \rangle c_{\gamma} c_{\delta}$$

Raimes | p.42 / Eq.2.117 → inclusive of spin labels



PCD TACS Unit 1 Select/Special Topics from 'Theory of Atomic Collisions & Spectroscopy'

24

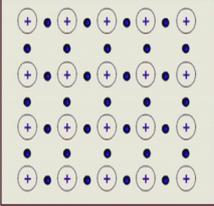
Now here again we will develop the complete expressions of the Hamiltonian including the spin labels using second quantized formalism. Using the field operators and also or the equivalently the creation and destruction operators. (Refer Slide Time: 17:19)

Hartree Fock Self Consistent Field for the Free Electron Gas

For FEG, the HF-SCF can be obtained ANALYTICALLY

- FEG → only many-electron system for which HF-SCF can be obtained ANALYTICALLY

'free'
in $V=0$
No interaction with any external field



What about the effect of the positive nuclei?

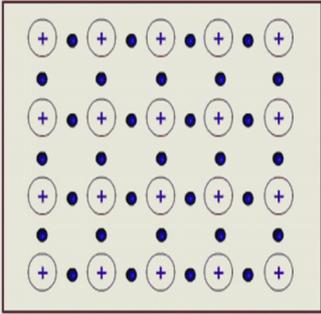
Fermi gas of electrons which interact only with each other.

NPTEL

PCD TACS Unit 1 Select/Special Topics from Theory of Atomic Collisions & Spectroscopy

25

And we will deal with; we will follow the Bohm Pines method in which what they did was to address the question of the electron gas in condensed matter. In which you have got electron gas which is smeared out in a metal for example. But there also is a positive charge so what they did was to smear out that positive charge throughout the volume of the metal. (Refer Slide Time: 17:48)





discrete positive charges in the nuclei considered smeared out, like jelly beans into a jellium.

Whole system: electrically neutral.

NPTEL

PCD TACS Unit 1 Select/Special Topics from Theory of Atomic Collisions & Spectroscopy

26

And that is what is called as a Jellium potentials. So, as if whatever charge was concentrated in the nuclei is smashed out and then you smear it out in the entire region of space. So, that is the system that is the electron gas in Jellium potential. The reason to do that is so that you deal with an electrically neutral system. (Refer Slide Time: 18:08)

electron gas in jellium potential $E_{HF} = E_{KE} + E_{exchange\ correlation}$ ← Adding both the terms

where $E_{KE} = 2 \frac{\hbar^2}{(2\pi\hbar)^3} \int_{p=0}^{p=p_f} p^2 dp \int_{\theta=0}^{\theta=\pi} \sin\theta d\theta \int_{\phi=0}^{\phi=2\pi} d\phi \left[\frac{\vec{p} \cdot \vec{p}}{2m} \right]$

and $E_{exchange\ correlation} = 2 \frac{\hbar^2}{(2\pi\hbar)^3} \int_{p=0}^{p=p_f} p^2 dp \int_{\theta=0}^{\theta=\pi} \sin\theta d\theta \int_{\phi=0}^{\phi=2\pi} d\phi \left[\frac{1}{2} \epsilon_{exchange}(\vec{p}) \right]$

For free electron gas in SCF jellium potential:

$\left[\frac{E_{HF}}{N} \right] = \left(\frac{2.21}{r_s^2} - \frac{0.916}{r_s} \right) Ryd$ r_s : Bohr units

Average HF energy per electron $H = \sum_{i=1}^N f(q_i) + \frac{1}{2} \sum_{i=1}^N \sum_{\substack{j=1 \\ i \neq j}}^N v(q_i, q_j)$

NPTEL PCD TACS Unit 1 Select/Special Topics from Theory of Atomic Collisions & Spectroscopy 27

And using this method you can first address the dynamics of this system in the Hartree Fock approximation in which you get a certain expression for the energy per particle which turns out to be what you find on the screen which is 2.21 upon r_s square and .916 upon r_s , r_s is like the average radius of an electron if you presume that all of these N electrons occupy a total amount of space of the condensed matter block itself. (Refer Slide Time: 18:46)

$H_{e-e} = \left[\frac{1}{2V} \sum_{\vec{k}} \sum_{\vec{p}} \sum_{\vec{q}=0} \sum_{\sigma_1} \sum_{\sigma_2} \left(\frac{4\pi}{q^2 + \mu^2} c_{\vec{k}+\vec{q}\sigma_1}^\dagger c_{\vec{p}-\vec{q}\sigma_2}^\dagger c_{\vec{p}\sigma_2} c_{\vec{k}\sigma_1} \right) \right]$

$H = H_{el} + H_b + H_{el-b}$ $\lim_{V \rightarrow \infty} \frac{E_{HF}}{N}$

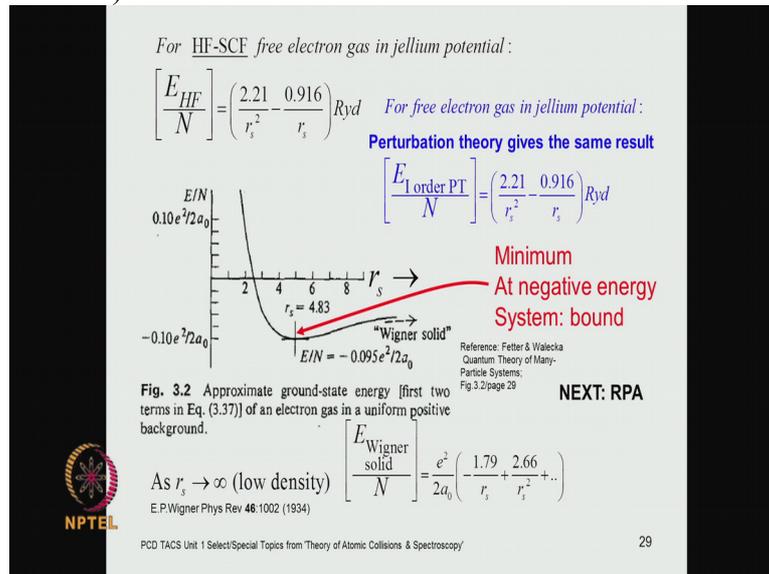
Hamiltonian for a bulk electron gas in a uniform positive background jellium potential

$H = \left[\sum_{\vec{k}} \sum_{\sigma} \frac{\hbar^2 \vec{k}^2}{2m} c_{\vec{k}\sigma}^\dagger c_{\vec{k}\sigma} \right] + \left[\frac{1}{2V} \sum_{\vec{k}} \sum_{\vec{p}} \sum_{\vec{q}=0} \sum_{\sigma_1} \sum_{\sigma_2} \left(\frac{4\pi}{q^2} c_{\vec{k}+\vec{q}\sigma_1}^\dagger c_{\vec{p}-\vec{q}\sigma_2}^\dagger c_{\vec{p}\sigma_2} c_{\vec{k}\sigma_1} \right) \right]$

NPTEL PCD TACS Unit 1 Select/Special Topics from Theory of Atomic Collisions & Spectroscopy 28

So, this is the expression that you get in the Hartree Fock approximation. But then you can go ahead and do it using the random phase approximation and to be able to do that you use the methods of second quantization. And keep track of all the interactions because the total Hamiltonian you can write in various pieces the electron, electron part, the electronic part. Then you have got the background which is the jellium and then there is also the interaction between the background and the electron system which is between the jellium and the

electronic system. And then you have to find out which if there is any cancellation of the terms and so on. So, we will do this part carefully.
(Refer Slide Time: 19:20)



And then we will ask if there are any corrections to the Hartree Fock expression and we do find that yes indeed.
(Refer Slide Time: 19:39)

$$H_0 = \sum_{i=1}^N \frac{p_i^2}{2m} + \frac{2\pi e^2}{V} \sum_{j=1}^N \sum_{i=1}^N \sum_{\substack{\vec{k} \\ \vec{k} \neq 0}} \frac{1}{k^2} e^{i\vec{k} \cdot (\vec{r}_i - \vec{r}_j)}$$

Quantum treatment
 $H_0 \psi = E \psi$

D. Bohm and D. Pines Phys. Rev. **82** 625 (1951)
D. Pines and D. Bohm Phys. Rev. **85** 338 (1952)
D. Bohm and D. Pines Phys. Rev. **92** 609 (1953)
D. Pines Reviews of Modern Physics **28** 184 (1956)

S Raimes 1957 Rep. Prog. Phys. **20** 1
The theory of plasma oscillations in metals

Method: transform the above Hamiltonian such that plasma oscillations appear explicitly as solutions of a set of Hamiltonians for simple harmonic oscillators for various values of \vec{k} with $k \leq k_{\text{max}} \approx \frac{\omega_p}{v_f} \leftrightarrow k_c$

PCD TACS Unit 1 Select/Special Topics from 'Theory of Atomic Collisions & Spectroscopy'

NPTEL

30

We do get corrections and these are the; this was the technique which was introduced by Bohm and Pines in the 1950's. So, there were very nice papers in the physical review during that period Raimes has got a nice review in the reports on progress in physics and of course the book by Raimes, which I like to refer to is a very good source for reading this particular information. So, what this technique?
(Refer Slide Time: 20:05)

$$H_0 = \sum_{i=1}^N \frac{p_i^2}{2m} + \frac{2\pi e^2}{V} \sum_{\substack{j=1 \\ j \neq i}}^N \sum_{\substack{k \\ k \neq 0}} \frac{1}{k^2} e^{i\vec{k} \cdot (\vec{r}_i - \vec{r}_j)}$$

$$H_0 = \sum_{i=1}^N \frac{p_i^2}{2m} + \frac{2\pi e^2}{V} \sum_{\substack{k \\ k \neq 0}} \frac{1}{k^2} \left(\sum_{i=1}^N e^{i\vec{k} \cdot \vec{r}_i} \sum_{\substack{j=1 \\ j \neq i}}^N e^{-i\vec{k} \cdot \vec{r}_j} \right)$$

Include the $j=i$ term, and then subtract its effect!

$$\rho_{\vec{k}} = \sum_{i=1}^N e^{-i\vec{k} \cdot \vec{r}_i}$$

$$\rho_{\vec{k}}^* = \sum_{j=1}^N e^{+i\vec{k} \cdot \vec{r}_j}$$

$j=i$ terms would give: $1+1+1+\dots+1 = N$

$$H_0 = \sum_{i=1}^N \frac{p_i^2}{2m} + \frac{2\pi e^2}{V} \sum_{\substack{k \\ k \neq 0}} \frac{1}{k^2} (\rho_{\vec{k}}^* \rho_{\vec{k}} - N)$$

NPTEL
 PCD TACS Unit 1 Select/Special Topics from 'Theory of Atomic Collisions & Spectroscopy' 31

What the Bohm Pines technique does is to transform the Hamiltonian into a set of new coordinates and new momenta. So, this is a method of coordinate transformation, canonical transformation of the Hamiltonian written in terms of new coordinates and momenta. This has to be done very systematically. (Refer Slide Time: 20:24)

$$H_0 = \sum_{i=1}^N \frac{p_i^2}{2m} + \frac{2\pi e^2}{V} \sum_{\substack{k \\ k \neq 0}} \frac{1}{k^2} (\rho_{\vec{k}}^* \rho_{\vec{k}} - N)$$

Transformation

$$H_{\vec{k}} = \frac{P_{\vec{k}}^\dagger P_{\vec{k}}}{2} + \frac{1}{2} \omega^2 Q_{\vec{k}}^\dagger Q_{\vec{k}}$$

Method: start with a 'model' Hamiltonian

$$H_1 = \sum_{\vec{k}(\vec{k}_x)} \frac{1}{2} P_{\vec{k}}^\dagger P_{\vec{k}} - M_{\vec{k}} P_{\vec{k}}^\dagger \rho_{\vec{k}} \quad \text{with } M_{\vec{k}} = \sqrt{\frac{4\pi e^2}{V k^2}}$$

$Q, P: \text{ NOT Hermitian} \rightarrow P_{\vec{k}}^\dagger = P_{-\vec{k}} \quad ; \quad Q_{\vec{k}}^\dagger = Q_{-\vec{k}}$

$$\rho_{\vec{k}} = \sum_{i=1}^N e^{-i\vec{k} \cdot \vec{r}_i} \quad \rho_{\vec{k}}^\dagger = \rho_{\vec{k}}^* = \sum_{i=1}^N e^{+i\vec{k} \cdot \vec{r}_i} = \rho_{-\vec{k}}$$

$H_1 \rightarrow \text{Hermitian}$

NPTEL
 PCD TACS Unit 1 Select/Special Topics from 'Theory of Atomic Collisions & Spectroscopy' 32

So, Bohm Pines came up with some very innovative transformation techniques and to set of new coordinates and momenta. (Refer Slide Time: 20:30)



$$H = H_{new} = \sum_{i=1}^N \frac{p_i^2}{2m} + \sum_{\vec{k}} \frac{1}{2} (p_{\vec{k}}^\dagger p_{\vec{k}} + \rho_{\vec{k}}^2 Q_{\vec{k}}^\dagger Q_{\vec{k}}) - \sum_{\vec{k}; \vec{k} \neq 0} \frac{2\pi e^2}{V k^2} N$$

$$+ H_{s,r} + H_{int} + K$$

"EXACT"

Raimis: Many Electron Theory
Eq. 4.58, page 58

$$H_{s,r} = \frac{1}{2} \sum_{\vec{k}; \vec{k} \neq 0}^{k > k_c} M_{\vec{k}}^2 (\rho_{\vec{k}}^\dagger \rho_{\vec{k}} - N)$$

$$H_{int} = -\frac{i}{2m} \sum_j \sum_{\vec{k}} M_{\vec{k}} Q_{\vec{k}} \vec{k} \cdot (2\vec{p}_j + \hbar \vec{k}) e^{-i\vec{k} \cdot \vec{r}_j}$$

"Random Phase Approximation"
"LINEARIZATION"

$$K \ll \frac{1}{2m} \sum_{\vec{k}} \sum_{\vec{\ell}} M_{-\vec{k}} M_{\vec{\ell}} (\vec{k} \cdot \vec{\ell}) \left\{ \sum_j (Q_{-\vec{k}} e^{i\vec{k} \cdot \vec{r}_j} \times Q_{\vec{\ell}} e^{-i\vec{\ell} \cdot \vec{r}_j}) \right\}$$

CPD TACS Unit 1 Select/Special Topics from Theory of Atomic Collisions & Spectroscopy' 33

In terms of which they were able to rewrite the new Hamiltonian in a set of completely new transformation which describes the original system however in terms of canonical transformations to new coordinates and momenta. So, when you do that you do get plenty of terms and they are quite complicated to handle.

But you can carry out certain approximations and using these approximations the final form of the Hamiltonian becomes very handy and it is very easily amenable to physical analysis. (Refer Slide Time: 21:18)



$$H = H_{new} = \sum_{i=1}^N \frac{p_i^2}{2m} + \sum_{\vec{k}} \frac{1}{2} (p_{\vec{k}}^\dagger p_{\vec{k}} + \rho_{\vec{k}}^2 Q_{\vec{k}}^\dagger Q_{\vec{k}}) - \sum_{\vec{k}; \vec{k} \neq 0} \frac{2\pi e^2}{V k^2} N$$

$$+ H_{s,r} + H_{int} + K$$

"EXACT"

Raimis: Many Electron Theory
Eq. 4.58, page 58

$$H_{s,r} = \frac{1}{2} \sum_{\vec{k}; \vec{k} \neq 0}^{k > k_c} M_{\vec{k}}^2 (\rho_{\vec{k}}^\dagger \rho_{\vec{k}} - N)$$

$$H_{int} = -\frac{i}{2m} \sum_j \sum_{\vec{k}} M_{\vec{k}} Q_{\vec{k}} \vec{k} \cdot (2\vec{p}_j + \hbar \vec{k}) e^{-i\vec{k} \cdot \vec{r}_j}$$

"Random Phase Approximation"
"LINEARIZATION"

$$K \ll \frac{1}{2m} \sum_{\vec{k}} \sum_{\vec{\ell}} M_{-\vec{k}} M_{\vec{\ell}} (\vec{k} \cdot \vec{\ell}) \left\{ \sum_j (Q_{-\vec{k}} e^{i\vec{k} \cdot \vec{r}_j} \times Q_{\vec{\ell}} e^{-i\vec{\ell} \cdot \vec{r}_j}) \right\}$$

CPD TACS Unit 1 Select/Special Topics from Theory of Atomic Collisions & Spectroscopy' 33

And that is done using this method of Bohm Pines and the approximation which is made is that of linearization. So, there are certain quadratic terms over here. So, the Q's so there is a Q here and a Q here so, there are quadratic terms in Q and these are the ones which are left out in a linearization process and one can argue as to what is the justification for this linearization. So, we will discuss all of these aspects and details in this unit. (Refer Slide Time: 21:47)

Raimes: Many Electron Theory, Eq.4.63, page 82

$$H = H_{\text{new}} = \sum_{\vec{k}; k < k_c} \frac{1}{2} (P_k^\dagger P_k + \omega_p^2 Q_k^\dagger Q_k) + \sum_{i=1}^N \frac{p_i^2}{2m} + H_{s,r} - \sum_{\vec{k}; k=0} \frac{2\pi e^2}{V k^2} N$$

Subsidiary condition: $(P_k)_{\text{new}} \psi_{\text{new}} = 0$ for $k < k_c$

What kind of a system does this Hamiltonian describe?

SHO Hamiltonian $H = \frac{1}{2} \left(\frac{p^2}{m} + m\omega^2 x^2 \right)$

Plasma oscillations

Quasi particles interacting via $H_{s,r}$.

A constant term that is part of the electron self-energy which not accounted for in the plasma oscillations.

Long range interaction is accounted for by PLASMONS, and the short range part that remains is a screened Coulomb interaction.

NPTEL

PCD TACS Unit 1 Select/Special Topics from Theory of Atomic Collisions & Spectroscopy 34

And we will introduce the random of phase approximation so, in the new set of coordinates and momenta generalized coordinates and new momenta the Hamiltonian for the many electron system in the background of Jellium potential can be written in three pieces one which looks like the Hamiltonian for an oscillator which gives you the explanation for the plasma oscillations you get in a many electron system.
(Refer Slide Time: 22:28)

Select/Special Topics in Atomic Physics



Unit 4 (8 lectures) Lectures 25 to 32

Feynman Diagram Methods

NPTEL

PCD TACS Unit 1 Select/Special Topics from Theory of Atomic Collisions & Spectroscopy 35

Then you have short-range interaction between these quasi particles and then you also have a part which is coming from the self energy of the electrons. So, we will conclude this discussion with the final result that we get from the Bohm Pines method of canonical transformations.
(Refer Slide Time: 22:35)

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

The above Hamiltonian \rightarrow
 \rightarrow not an explicit function of time

If we can treat **this term** **as if** it has a time-dependence, then the mathematical procedure that would enable us to do so, would also provide access to powerful methods using the INTERACTION (Dirac) "PICTURE".



PDD TACS Unit 1 Select/Special Topics from Theory of Atomic Collisions & Spectroscopy / 36

Then we will introduce the Feynman diagram methods and for that we will essentially make use of the interaction picture, quantum mechanics in the interaction picture. So, we will introduce the Dirac picture description of a many electron Hamiltonian. (Refer Slide Time: 22:55)

$H_0\Phi_0 = E_0\Phi_0$ Gell-Mann and Low theorem

$$H = (H_0 + e^{\alpha t} H_1) \xrightarrow{t \rightarrow -\infty} H_0$$

Question: How do we get eigenstate of $H = H_0 + H_1$?

$\psi_i(\vec{r}, t=0) = \Psi_0 = U_\alpha(t=0, t=-\infty)\Phi_0$

If $\lim_{\alpha \rightarrow 0} \frac{U_\alpha(0, -\infty)|\Phi_0\rangle}{\langle \Phi_0 | U_\alpha(0, -\infty) | \Phi_0 \rangle} \equiv \frac{|\Psi_0\rangle}{\langle \Phi_0 | \Psi_0 \rangle}$ exists, RATIO

then it is an eigenstate of $H = H_0 + H_1$; $t_0 \rightarrow -\infty$

i.e. $H \left| \frac{|\Psi_0\rangle}{\langle \Phi_0 | \Psi_0 \rangle} \right\rangle = E \left| \frac{|\Psi_0\rangle}{\langle \Phi_0 | \Psi_0 \rangle} \right\rangle$ For PROOF, see: Fetter & Walecka Quantum Theory of Many-Particle Systems, page 61



PDD TACS Unit 1 Select/Special Topics from Theory of Atomic Collisions & Spectroscopy / 37

And then we will make use of the Gell-Mann and Low theorem to relate the solutions inclusive of the correlations of the many electron system. In terms of a solvable part which excludes the electron-electron interactions. So, it is some sort of a perturbative approach but it is quite different also and it allows us to use this chronological evolution of the system from an uncorrelated system to a correlated system. (Refer Slide Time: 23:14)

$$H = (H_0 + e^{\alpha t} H_1) \xrightarrow{t \rightarrow -\infty} H_0$$

$$H_0 |\Phi_0\rangle = E_0 |\Phi_0\rangle$$

$$H \frac{|\Psi_0\rangle}{\langle \Phi_0 | \Psi_0 \rangle} = E \frac{|\Psi_0\rangle}{\langle \Phi_0 | \Psi_0 \rangle}$$

$$E - E_0 = \Delta E = ?$$

$$\Delta E_{\text{Adiabatic Hypothesis}} = \lim_{\alpha \rightarrow 0} i\hbar \left[\frac{\partial}{\partial t} \log \langle \Phi_0 | U_\alpha(t, -\infty) | \Phi_0 \rangle \right]_{t=0}$$

Correspondence? $\Delta E_{\text{Rayleigh Schrodinger Perturbation Theory}} = ?$

What is the form of the time evolution operator?

NPTEL
 PCD TACS Unit 1 Select/Special Topics from Theory of Atomic Collisions & Spectroscopy/ 38

So, that we can see exactly what is the role of these correlations and how are these to be addressed. So, you can approach this from the point of view of an adiabatic hypothesis in which you introduce the electron-electron correlations adiabatically through a mathematical switch. But then you can compare the results with what you can get through the formal Reyleigh Schrodinger perturbation theory. (Refer Slide Time: 23:45)

$$\Delta E = \Delta E^{(1)} + \Delta E^{(2)} + \Delta E^{(3)} + ..$$

$$\Delta E = \lim_{\alpha \rightarrow 0} i\hbar \frac{\partial}{\partial t} \left[\left((A_1 + A_2 + A_3 + \dots) - \frac{1}{2} \left(\begin{array}{l} A_1^2 + A_2^2 + A_3^2 + \dots \\ + A_1 A_2 + A_1 A_3 + A_2 A_3 + \dots \\ + A_2 A_1 + A_2 A_3 + A_1 A_4 + \dots \end{array} \right) \right) + \frac{1}{3} \left(\begin{array}{l} A_1^3 + A_2^3 + A_3^3 + \dots \\ + A_1 A_2^2 + A_1 A_3^2 + A_2 A_4^2 + \dots \\ + A_2 A_1^2 + A_2 A_3^2 + A_2 A_4^2 + \dots \end{array} \right) - \dots \right]_{t=0}$$

Adiabatic 'switch' on the correlation / perturbation

Chronological operator

$$A_n = \langle \Phi_0 | U_n | \Phi_0 \rangle$$

$$= \left\langle \Phi_0 \left| \left(\frac{-i}{\hbar} \right)^n \frac{1}{n!} \int_{-\infty}^t dt_1 \int_{-\infty}^{t_1} dt_2 \dots \int_{-\infty}^{t_{n-1}} dt_n T [H_1(t_1) H_1(t_2) \dots H_1(t_n)] \right| \Phi_0 \right\rangle$$

NPTEL
 PCD TACS Unit 1 Select/Special Topics from Theory of Atomic Collisions & Spectroscopy/ 39

And when you develop this formalism it turns out that the; you really get infinite terms and a multiplicity of them. So, there are just too many terms the whole description becomes quite complicated. You have the chronological operator which orders all the operators with the latest operators to the left and so on. So, this so the whole analysis is quite complicated. (Refer Slide Time: 24:14)

$$A_n = \langle \Phi_0 | U_n | \Phi_0 \rangle = \left(\frac{-i}{2\hbar} \right)^n \left\langle \Phi_0 \left| \int_{t_0}^{t_1} \left[\langle ij | \langle l | \dots \langle uv | v | \rangle x \right] \right. \right. \\ \left. \left. \times \frac{1}{[i(\Delta_1 + \Delta_2 + \dots + \Delta_n) + (n-1)\alpha]} \times \langle \Phi_0 | c_i^\dagger c_j c_k c_l c_p^\dagger c_q c_s \dots c_a c_b c_c | \Phi_0 \rangle \right. \right. \\ \left. \left. \times \dots \times \frac{1}{i\Delta_n + \alpha} \times \frac{e^{i(\Delta_1 + \Delta_2 + \dots + \Delta_n) + n\alpha} t} { [i(\Delta_1 + \Delta_2 + \dots + \Delta_n) + n\alpha]} \right. \right. \\ \left. \left. \right. \right.$$

But then it is a Feynman diagrams which make them easy to analyze okay. Because all of these terms you can handle in a very compact and beautiful manner in a very elegant manner by introducing Feynman diagrams which is what we will do in this unit. (Refer Slide Time: 24:31)

Principal elements of a Feynman diagram/graph

particle lines point upwards hole lines point downwards

It does not matter whether these lines lean toward left or right; or do not lean at all...

Wiggly lines: mediators of the interaction → photons

Vertex: indicates where the interaction occurs

particle and hole lines go *in* or *out* of a vertex.....

....depending on particle/hole creation/destruction.....

So, we will define these diagrams they are based on certain conventions. So, an arrow pointing upward or downward has got a different meaning whether these are the particle lines or the hole lines of course it depends on what kind of convention you have for the time axis whether time is flowing from the bottom to the top are from left to right. So, there are certain conventions which you have to define. (Refer Slide Time: 25:08)

FIRST ORDER FEYNMAN DIAGRAMS



$\checkmark \Delta_1 = (\omega_i + \omega_j - \omega_l - \omega_k)$

for some particular i, j, k, l \checkmark

$$A_1 = \langle \Phi_0 | U_1 | \Phi_0 \rangle$$

$$= \frac{-i}{2\hbar} \sum_{i,j,k,l} \langle ij | v | lk \rangle \langle \Phi_0 | c_i^\dagger c_j^\dagger c_k c_l | \Phi_0 \rangle \frac{e^{i(\Delta_1 + \alpha)t}}{(i\Delta_1 + \alpha)}$$

$\langle ij | v | lk \rangle \langle \Phi_0 | c_i^\dagger c_j^\dagger c_k c_l | \Phi_0 \rangle$

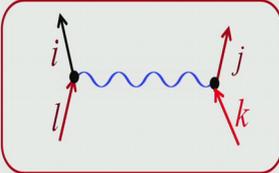


PCD TACS Unit 1 Select/Special Topics from 'Theory of Atomic Collisions & Spectroscopy'

42

And then you can define the particle creation and destruction in terms of these arrows which go into a vertex are out of a vertex and so on. So, we will define these conventions and then they will help us analyze the terms which go into the many-body electron correlation.
(Refer Slide Time: 25:24)

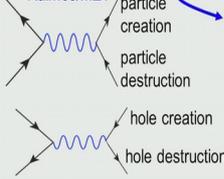
Consider: $\epsilon_i, \epsilon_j > \epsilon_F$
 $\epsilon_l, \epsilon_k > \epsilon_F$



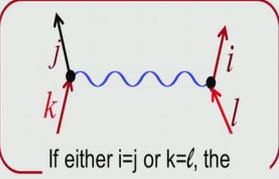
$c_i^\dagger c_j^\dagger c_k c_l \equiv a_i^\dagger a_j^\dagger a_k a_l$

Interchange vertices
 $V_{left} \square V_{right}$

Fig. 7.8/page123
Raimis/MET



\checkmark *equivalent* \checkmark



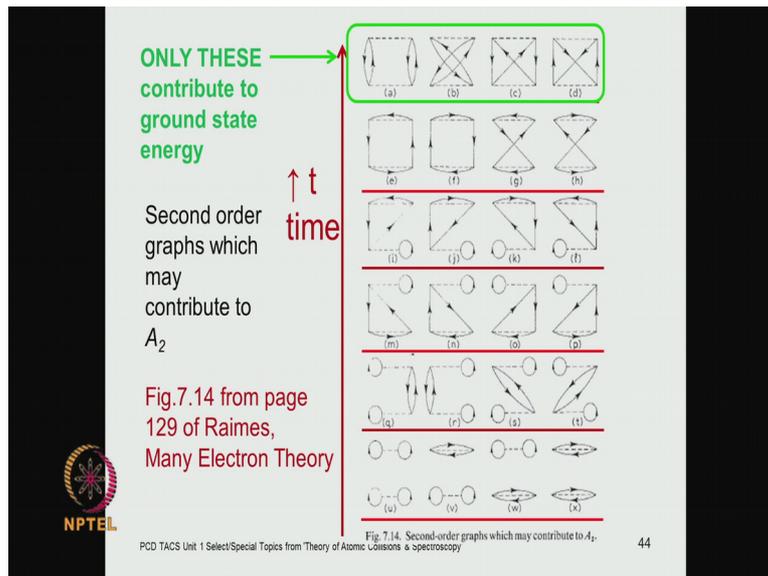
If either $i=j$ or $k=l$, the term becomes zero



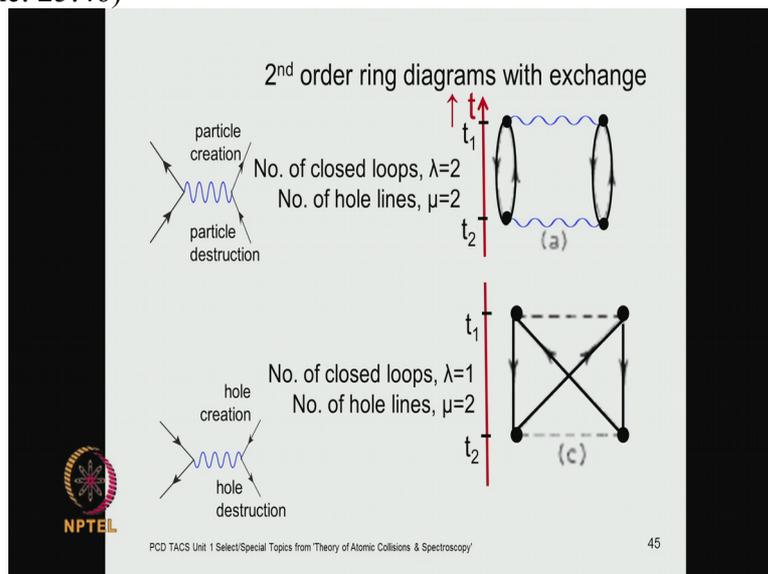
PCD TACS Unit 1 Select/Special Topics from 'Theory of Atomic Collisions & Spectroscopy'

43

So, that we can describe them in terms of these very nice very beautiful elegant pictures known as Feynman diagrams. So, we will spend some time discussing the first our order diagrams.
(Refer Slide Time: 25:28)



Then we will also introduce the second order diagrams and also the third order diagrams. So, that we get some sort of a familiarity with this technique we will also learn to recognize which diagrams are equivalent, which are not equivalent, which are the fundamental ones, which need to be used which are connected, which are not connected. (Refer Slide Time: 25:46)



And then how when you do many body theory you can select a group of diagrams to address. So that you can restrict your attention to certain correlations which you think are important for your study and the RPA the random phase approximation comes through one of these techniques or retaining only these ring diagrams and the corresponding exchange. So, some of these things we will discuss in the context of the Feynman diagrams. (Refer Slide Time: 26:12)

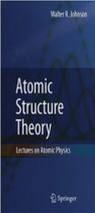
PHYSICAL REVIEW A VOLUME 20, NUMBER 3 SEPTEMBER 1979

Multichannel relativistic random-phase approximation for the photoionization of atoms

W. R. Johnson
Department of Physics, University of Notre Dame, Notre Dame, Indiana 46556

C. D. Lin
Department of Physics, Kansas State University, Manhattan, Kansas 66506
 (Received 5 January 1979)

A multichannel relativistic random-phase approximation (RRPA) for the photoionization of atoms is presented. The RRPA equations are obtained by generalizing the nonrelativistic time-dependent Hartree-Fock equations using the Dirac-Breit Hamiltonian to describe the atomic electrons. The angular decomposition of the RRPA equations to a set of coupled equations for the radial wave functions is given, and the radiative-transition operators are developed for arbitrary electric and magnetic multipoles. Formulas are obtained for the total photoionization cross sections and angular distributions, including all multipoles. The method of constructing multichannel solutions from the RRPA radial wave functions is described and various ways of choosing approximate potentials for the photoelectron are given.




PCD TACS Unit 1 Select/Special Topics from 'Theory of Atomic Collisions & Spectroscopy'

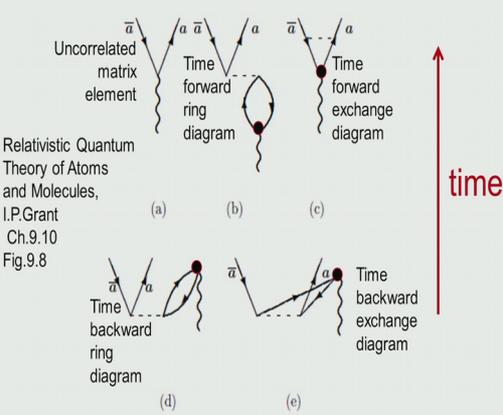
NPTEL

46

I will also spend some time in describing yet another way of getting the RPA like I mentioned there is a Bohm Pines method of getting the random phase approximation. There is basically it is a linearization technique. So, even in the diagrammatic perturbation theory, if you keep the ring diagrams again you get an equivalent or what is RPA.

But you can get it also by carrying out a linearization of the time dependent Dirac Hartree Fock and this is the technique that was done that was used by Dalgarno and Victor for the non relativistic many body problem and by Dalgarno and Walter Johnson for the relativistic case which is known as a linearization of the time dependent Dirac Hartree Fock method or which is equivalently called as the relativistic random phase approximations. So, I will provide some introduction to that.

(Refer Slide Time: 27:17)



Relativistic Quantum Theory of Atoms and Molecules, I.P.Grant Ch.9.10 Fig.9.8

Fig. 9.8. Lowest order Feynman diagrams contributing to the RRPA transition matrix element: (a) uncorrelated matrix element, (b,c) positive frequency final state correlations, (d,e) ground state correlations. Time increases up the page. Solid lines: electrons/holes in the DHF basis. Dashed lines: instantaneous electron-electron interaction. Wiggly lines: photons. a, \bar{a} : particle/hole labels.

PCD TACS Unit 1 Select/Special Topics from 'Theory of Atomic Collisions & Spectroscopy'

NPTEL

47

(Refer Slide Time: 27:26)

Select/Special Topics in Atomic Physics



Unit 5 (3 lectures) Lectures 33 to 35

Quantum Collision Theory – Part 2

Lippman-Schwinger Equation

Born Approximations

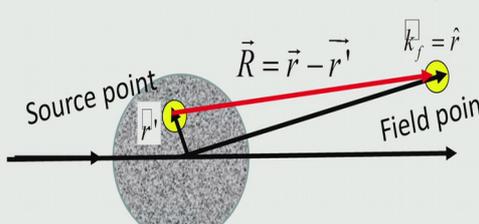
Coulomb scattering



PCD TACS Unit 1 Select/Special Topics from 'Theory of Atomic Collisions & Spectroscopy' 48

And then you get the relativistic RPA diagrams which as you can see from this are again basically focused on the ring diagrams which is a central feature of the RPA. In the unit 5 we will you get back to quantum collisions and I like I said that in principle one can study this after the first unit in which we would have studied the Levinson's theorem and so on. So, in this unit we will introduce the Lippman Schwinger equation which is the integral equation of potential scattering. We will also do the Born approximations. (Refer Slide Time: 27:50)

Green's function.

$$k\hat{r} = k\hat{k}_f = \vec{k}_f$$


Source point Field point

$$\vec{R} = \vec{r} - \vec{r}'$$

$$\vec{k}_f = \hat{r}$$

$\vec{r} = r\hat{e}_r$ ← Position vector of the 'field' point

$\vec{r}' = r'\hat{e}_{r'} = r'\hat{e}_{k_f}$ ← Position vector of the 'source' point in the region of the scatterer.



PCD STITACS Unit 1 Select/Special Topics from 'Theory of Atomic Collisions & Spectroscopy' 49

We will also do Coulomb scattering. So, we will introduce methods in which the Green's functions are used. So, there is a certain causality which is referred to over here. (Refer Slide Time: 28:05)

$$\left[\frac{(-i\hbar\vec{\nabla})^2}{2m} + V(\vec{r}) \right] \psi(\vec{r}) = E\psi(\vec{r}) \quad \leftarrow \text{Schrodinger equation}$$

$$[\vec{\nabla}^2 + k^2]G_0(k, \vec{r}, \vec{r}') = \delta^3(\vec{r} - \vec{r}')$$

We shall see that

$$\psi_{\vec{k}_i}^-(\vec{r}) = \phi_{\vec{k}_i}^-(\vec{r}) + \iiint d^3\vec{r}' G_0(k, \vec{r}, \vec{r}') U(\vec{r}') \psi_{\vec{k}_i}^-(\vec{r}')$$
 is a solution of the Schrodinger equation

↑ Green's function is to be determined according to appropriate boundary conditions.

"CATCH 22" ?


 PCD STTACS Unit 1 Select/Special Topics from 'Theory of Atomic Collisions & Spectroscopy' 50

We will write the Lippman Schwinger equation and we will find that it is amenable to an iterative solution because unless you make some approximation you cannot go too far with the Lippman Schwinger equation itself because it generates a catch-22 type of situation because you get a solution in terms of the problem. So, to be able to handle that you can develop certain approximation methods. (Refer Slide Time: 28:27)

$$G_0^+(\vec{R}) = \frac{-1}{16\pi^2 Ri} [2\pi i e^{ikR}] + \frac{1}{16\pi^2 Ri} [-2\pi i e^{ikR}]$$

$$G_0^+(\vec{R}) = \frac{-e^{ikR}}{4\pi R}$$
Outgoing boundary conditions incorporated

$$\psi_{\vec{k}_i}^-(\vec{r}) = \phi_{\vec{k}_i}^-(\vec{r}) + \iiint d^3\vec{r}' G_0(k, \vec{r}, \vec{r}') U(\vec{r}') \psi_{\vec{k}_i}^-(\vec{r}')$$

↑ Lippman-Schwinger ↑ equation for potential scattering.

↑ Green's function is to be determined according to appropriate boundary conditions.

$$\psi_{\vec{k}_i}^+(\vec{r}) = \phi_{\vec{k}_i}^+(\vec{r}) + \iiint d^3\vec{r}' G_0^+(k, \vec{r}, \vec{r}') U(\vec{r}') \psi_{\vec{k}_i}^+(\vec{r}')$$


 PCD TACS Unit 1 Select/Special Topics from 'Theory of Atomic Collisions & Spectroscopy' 51

And these approximation methods with reference to appropriate boundary conditions of the collision problem they let you choose what would be the appropriate Green's function that goes in the integral expression of the Lippman Schwinger equation. (Refer Slide Time: 28:45)

$$\psi_{\vec{k}_i}^+(\vec{r}) = \phi_{\vec{k}_i}(\vec{r}) + \iiint d^3\vec{r}' G_0^+(k, \vec{r}, \vec{r}') U(\vec{r}') \psi_{\vec{k}_i}^+(\vec{r}')$$

0th order solution: $\psi_{\vec{k}_i}^{+(0)}(\vec{r}) = \phi_{\vec{k}_i}(\vec{r}) + 0 = (2\pi)^{-3/2} e^{i\vec{k}_i \cdot \vec{r}}$

1st order :

$$\psi_{\vec{k}_i}^{+(1)}(\vec{r}) = \phi_{\vec{k}_i}(\vec{r}) + \iiint d^3\vec{r}' G_0^+(k, \vec{r}, \vec{r}') U(\vec{r}') \psi_{\vec{k}_i}^{+(0)}(\vec{r}')$$

2nd order :

$$\psi_{\vec{k}_i}^{+(2)}(\vec{r}) = \phi_{\vec{k}_i}(\vec{r}) + \iiint d^3\vec{r}' G_0^+(k, \vec{r}, \vec{r}') U(\vec{r}') \psi_{\vec{k}_i}^{+(1)}(\vec{r}')$$

nth order :

$$\psi_{\vec{k}_i}^{+(n)}(\vec{r}) = \phi_{\vec{k}_i}(\vec{r}) + \iiint d^3\vec{r}' G_0^+(k, \vec{r}, \vec{r}') U(\vec{r}') \psi_{\vec{k}_i}^{+(n-1)}(\vec{r}')$$



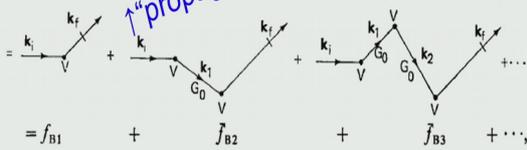
PCD TACS Unit 1 Select/Special Topics from Theory of Atomic Collisions & Spectroscopy/

So, when you choose the property in Green's function you get a series of approximation which are known as the Born approximation. So, there is a first order Born approximation the second order Born approximation and then nth ordered Born approximation. So, you will be introduced to this Born series of approximations.
 (Refer Slide Time: 29:00)

$$f_{B_n}(\hat{k}_i, \hat{k}_f) = \sum_{j=1}^n \bar{f}_{B_j} \quad f_{B_n}(\hat{k}_i, \hat{k}_f) = \sum_{j=1}^n \bar{f}_{B_j}$$

$$\psi_{\vec{k}_i}^{+(n)}(\vec{r}) = \phi_{\vec{k}_i}(\vec{r}) + \iiint d^3\vec{r}' G_0^+(k, \vec{r}, \vec{r}') U(\vec{r}') \psi_{\vec{k}_i}^{+(n-1)}(\vec{r}')$$

$$\bar{f}_{B_n} = \text{Green's function "propagator"} \uparrow \text{Born series} \quad \bar{f}_{B_1} = f_{B_1}$$



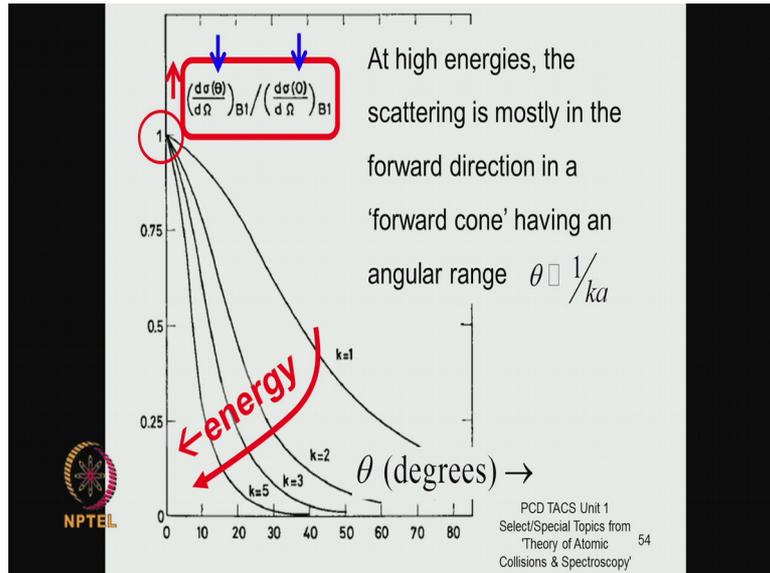
$$= f_{B1} + \bar{f}_{B2} + \bar{f}_{B3} + \dots$$



Multiple scattering series Ref.: Joachain/Eq.8.43

PCD TACS Unit 1 Select/Special Topics from Theory of Atomic Collisions & Spectroscopy/

So, we will spend some time discussing this and as you see most of this discussion will be based on Joe Shane's book quantum collision theory.
 (Refer Slide Time: 29:13)



And we will also discuss what happens in the Born approximations, How is it suitable in the high energy? What happens in the high energy range is the first Born approximation good enough.

(Refer Slide Time: 29:26)

$$\sigma_{total} = \frac{4\pi}{k} [\text{Im } f(0)] \quad \text{OPTICAL THEOREM}$$

Bohr-Peierls-Placzek relation
Reference: STITACS U1 L04

$$\text{Im } f_{B1}(\theta = 0) = 0$$

"non-linearity"

$$\sigma_{B1}^{Total} = \frac{4\pi}{k} [\text{Im } f_{B2}(\theta = 0)]$$

$$\iint d\Omega |f_{B1}(\hat{\Omega})|^2 = \frac{4\pi}{k} \text{Im } f_{B2}(\theta = 0)$$

Expand σ and f in Born series powers of the potential and consider corresponding powers in the expression for the optical theorem.

PCD STITACS Unit 1 Select/Special Topics from 'Theory of Atomic Collisions & Spectroscopy' 55

Is the optical theorem satisfied in the Born approximation or do you get a certain non-linearity over there. So, all of these questions we will take up in this unit.

(Refer Slide Time: 29:37)

Coulomb scattering

$$\left[\frac{(-i\hbar\nabla)^2}{2m} - \frac{(Z_1 e)(Z_2 e)}{r} \right] \psi(\vec{r}) = E\psi(\vec{r}) \quad \left| E = \frac{\hbar^2 k^2}{2m} > 0 \right.$$

$$\left[\nabla^2 + k^2 + \frac{2\gamma k}{r} \right] \psi(\vec{r}) = 0 \quad \left| m = \frac{m_1 m_2}{m_1 + m_2} \right.$$

$$\gamma = \frac{Z_1 Z_2 e^2 m}{\hbar^2 k} = \frac{Z_1 Z_2 e^2}{\hbar v} = \frac{\alpha c Z_1 Z_2}{v} \quad \left| \alpha = \frac{e^2}{\hbar c} \right.$$

$\gamma > 0 \leftrightarrow$ attractive potential

$(x, y, z) \rightarrow (\rho, \phi, z) \rightarrow (r, \theta, \phi)$

Cartesian Cylindrical Polar Spherical Polar

$$\rho^2 + z^2 = r^2$$

$$\rho^2 = r^2 - z^2 = (r+z)(r-z)$$

$\rightarrow (z, w, \phi)$
 Parabolic coordinates
 $w = r - z$
 $= r(1 - \cos\theta)$

PCD TACS Unit 1 Select/Special Topics from Theory of Atomic Collisions & Spectroscopy 56

We will also discuss Coulomb scattering and the Coulomb problem is a very peculiar problem because the usual methods which we discuss in quantum collisions do not apply directly to the 1 over r potential. So, this problem is addressed using a new set of coordinate system known as the parabolic coordinates.
 (Refer Slide Time: 30:02)

complex-s plane

$u = i\kappa(1 - \cos\theta)$
 $= i\kappa ; \kappa > 0$

$$s = s_0 + i\kappa$$

$s \neq 0$; rather $s = s_0$

$$s = s_0$$

$s = ut$
 $e^{st} = e^s \rightarrow 0$

Asymptotic limit:
 $u \rightarrow \infty$

On C_2 , $s = -s_0 + i(\kappa \pm \varepsilon)$

$$\int_{\bar{C}} \equiv \int_{C_1} + \int_{C_2}$$

On C_1 , $s = -(s_0 \pm i\varepsilon)$

PCD TACS Unit 1 Select/Special Topics from Theory of Atomic Collisions & Spectroscopy 57

So we will solve the problem of Coulomb scattering in parabolic coordinates using methods of contour integration and branch cuts.
 (Refer Slide Time: 30:08)

$$\psi(\vec{r}) = 2\pi i A e^{\frac{\gamma}{2}} g_1(\gamma) \left\{ e^{i[kz - \gamma \ln k(r-z)]} + \frac{\gamma}{2k \sin^2 \frac{\theta}{2}} e^{i\Theta(\gamma)} \frac{e^{i[kr + \gamma \ln k(r-z)]}}{r} \right\}$$

$r-z = r - r \cos \theta = r(1 - \cos \theta) = r \left(2 \sin^2 \frac{\theta}{2} \right)$ †Eq. 7.13.30
p.441/Sakurai/MQM

$$\psi(\vec{r}) \rightarrow e^{i[kz - \gamma \ln k(r-z)]} + f_c(k, \theta) \frac{e^{ikr} e^{i\gamma \ln(2kr)}}{k(r-z)}$$

$$f_c(k, \theta) = \frac{\gamma}{2k \sin^2 \frac{\theta}{2}} e^{i\left\{ \Theta(\gamma) + 2\gamma \ln \sin \frac{\theta}{2} \right\}}$$

←Eq. 7.13.31
p.441/Sakurai/MQM

$$\frac{d\sigma}{d\theta} = |f_c(k, \theta)|^2 = \frac{\gamma^2}{4k^2 \sin^4 \frac{\theta}{2}} \quad \leftarrow \text{Rutherford formula}$$

58

PCD TACS Unit 1 Select/Special Topics from 'Theory of Atomic Collisions & Spectroscopy'

So, we will get the solutions which will give us the Coulomb logarithmic phase shift and also the expression for the scattering cross section. Which turns out to be the same as you get in the Born approximation or for that matter also in classical mechanics. So, it turns out that so this is interesting coincidence that you get the same result for the scattering cross section in classical mechanics in the Born approximation and also in the complete quantum mechanical solution to the Coulomb problem.
(Refer Slide Time: 30:39)

Select/Special Topics in Atomic Physics



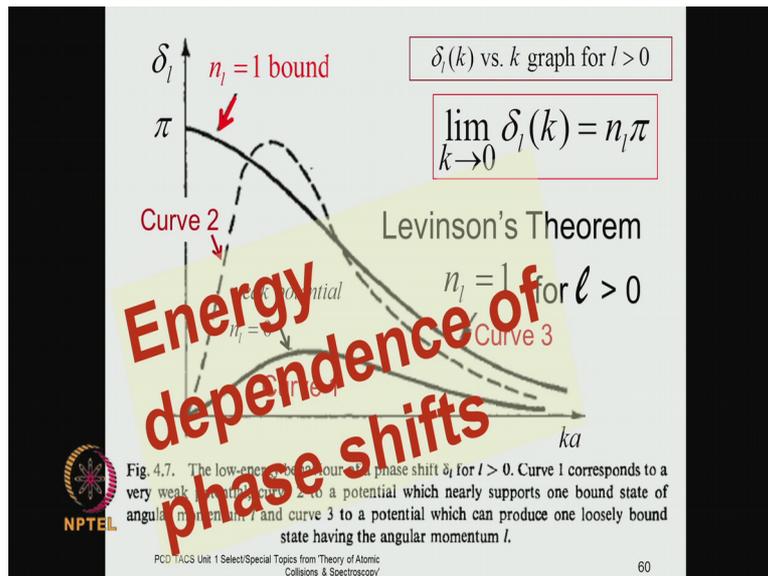
Unit 6 (4 lectures) Lectures 36 to 39

Quantum Collision Theory – Part 3
Resonances in Quantum Collisions

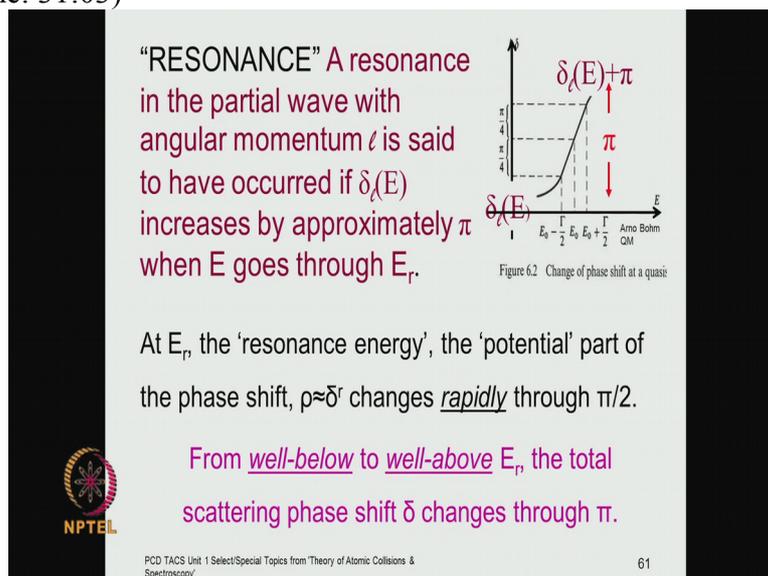
59

PCD TACS Unit 1 Select/Special Topics from 'Theory of Atomic Collisions & Spectroscopy'

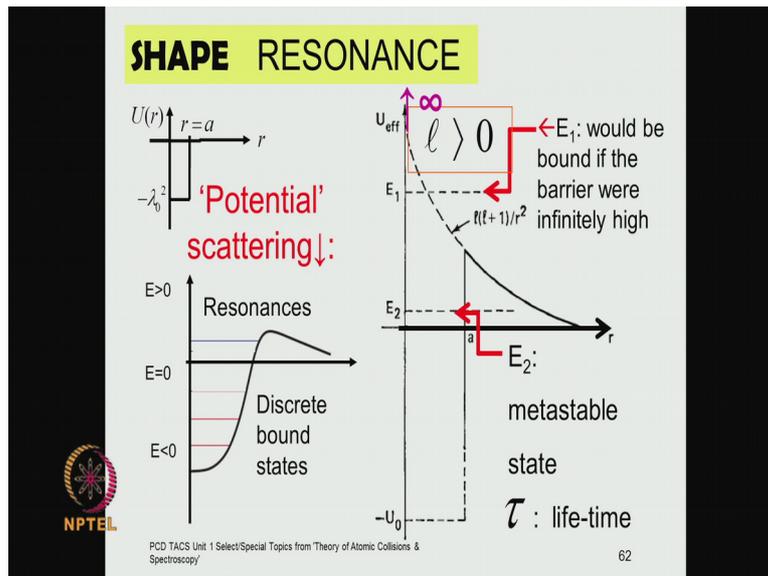
So, that will bring us to the next unit which will be on resonances in quantum collisions.
(Refer Slide Time: 30:47)



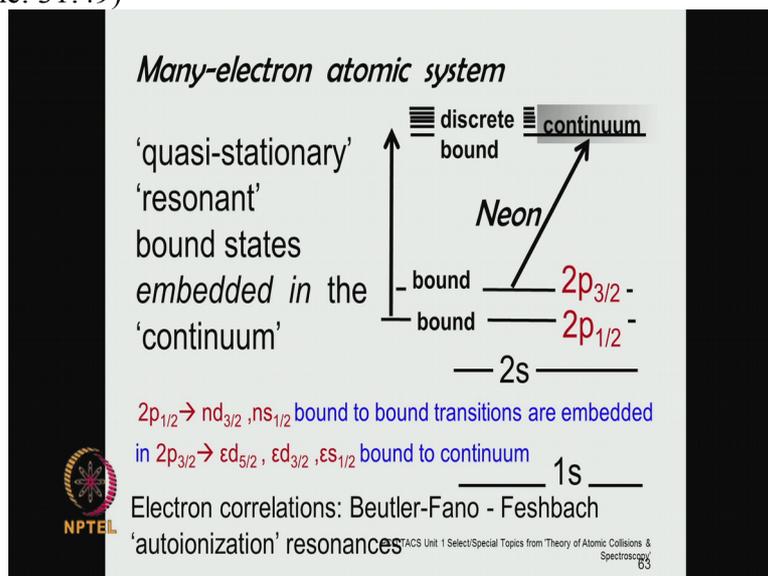
Because what happens is when you do a phase shift analysis the phase shifts, the scattering phase shifts they change somewhat rapidly in the vicinity of a resonance. So, we will discuss the energy dependence of the phase shifts.
(Refer Slide Time: 31:03)



And we will see that these phase shifts they change rather rapidly in the vicinity of resonance and so if you have a resonance at this energy then from slightly below the resonance to slightly above the resonance the phase shift undergoes a major change through pi. So, we will discuss and try to understand resonances in terms of how the scattering phase shift changes in the vicinity of resonance.
(Refer Slide Time: 31:42)



We will also discuss resonances of different kinds. So, broadly speaking there categorized either a shape resonances or as Fano Feshbach resonances. So we will describe both of them the shape resonances are because of the nature of the shape of the potential itself. (Refer Slide Time: 31:49)



And the Fano Feshbach resonance takes place when you have a quasi-stationary state. You have got a discrete state which is embedded in the continuum. So, you have got a resonance between a bound state, bound to bound excitation and a bound to continuum transition like ionization as you could have in the Butler Fano resonance or the autoionization resonances. (Refer Slide Time: 32:14)

Ugo Fano
Physical Review
Vol. 124 Number 6
December 15,
1961
p. 1866 to 1878



Configuration interaction in a many-electron system

- bound-bound
- bound-continuum

PHYSICAL REVIEW VOLUME 124, NUMBER 6 DECEMBER 15, 1961

Effects of Configuration Interaction on Intensities and Phase Shifts*

Ugo Fano
1912-2001

U. FANO
National Bureau of Standards, Washington, D. C.
(Received July 14, 1961)

The interference of a discrete autoionized state with a continuum gives rise to characteristically asymmetric peaks in excitation spectra. The earlier qualitative interpretation of this phenomenon is extended and revised. A theoretical formula is fitted to the shape of the $22p^1P$ resonance of He observed in the inelastic scattering of electrons. The fitting determines the parameters of the $22p^1P$ resonance as follows: $E=60.1$ eV, $\Gamma\sim 0.04$ eV, $f\sim 2$ to 4×10^{-3} . The theory is extended to the interaction of one discrete level with two or more continua and of a set of discrete levels with one continuum. The theory can also give the position and intensity shifts produced in a Rydberg series of discrete levels by interaction with a level of another configuration. The connection with the nuclear theory of resonance scattering is indicated.

PCD TACS Unit 1 Select/Special Topics from Theory of Atomic Collisions & Spectroscopy/ 64



So, in particular I think this is a topic which I hope all of you will enjoy very much because we will work through Fano's very famous paper this has received more citations and a lot of other papers which perhaps you might know better. But then the actual citations to this paper are far too many.

This is a very important paper in physics not just in atomic physics but it has got applications across physics in various disciplines Condensed matter physics, Molecular physics whatnot. (Refer Slide Time: 32:52)

$$\sigma_{tot} = \frac{4\pi}{k^2} \left[\sum_{l=0}^{\infty} (2l+1) \left[\sin^2 \xi_l(k) + \frac{\frac{1}{4}\Gamma^2}{(E_r - E)^2 + \frac{1}{4}\Gamma^2} + 2 \operatorname{Re} \sin \xi_l(k) \left(\frac{e^{i\xi_l(k)}}{E_r - E - \frac{1}{2}i\Gamma} \right) \right] \right]$$

Sum of contributions from all partial waves

$$\sigma_l = \frac{4\pi}{k^2} (2l+1) \left[\underbrace{\sin^2 \xi_l(k)}_{\text{'pure' background part}} + \underbrace{\frac{\frac{1}{4}\Gamma^2}{(E_r - E)^2 + \frac{1}{4}\Gamma^2}}_{\text{'pure' resonance part}} + 2 \sin \xi_l(k) \frac{1}{2} \Gamma \operatorname{Re} \left(\frac{e^{i\xi_l(k)}}{E_r - E - \frac{1}{2}i\Gamma} \right) \right]$$

'interference' part

Joachim, Quantum Collisions Theory, Eq. 4.223, page 98
Arno Bohm, Quantum Mechanics, Eq. 9.1, page 439
Bransden & Joachain, Physics of Atoms & Molecules, Eq. 12.137, page 598

PCD TACS Unit 1 Select/Special Topics from Theory of Atomic Collisions & Spectroscopy/ 65

Next: Fano-Feshbach resonance parameters



So, we will deal with this paper so we will arrive at a general expression for the Bright Wigner formula for resonances. In which the scattering cross section for the lth partial wave can be written separately in terms of the background part, the resonance part and the interference part between the resonance part and the background part. (Refer Slide Time: 33:13)

Select/Special Topics in Atomic Physics



Unit 7 (4 lectures)

Lectures 40 to 43

Quantum Collision Theory – Part 4

Fano-Feshbach and Shape Resonances; Life times and time delay in scattering



And then we will do what is known as a shape analysis of these resonance profiles. So, that can be done using Fano's methods.

(Refer Slide Time: 33:21)

$$\sigma_l = \frac{4\pi}{k^2} (2l+1) \left[\underbrace{\sin^2 \xi_l(k)}_b + \underbrace{\frac{\frac{1}{4}\Gamma^2}{(E_r - E)^2 + \frac{1}{4}\Gamma^2}}_r + 2 \sin \xi_l(k) \underbrace{\frac{1}{2}\Gamma \operatorname{Re} \left(\frac{e^{i\delta_l(k)}}{E_r - E - \frac{1}{2}i\Gamma} \right)}_i \right]$$

FANO parameters

$$\varepsilon = -\cot \delta_l^r(k) \quad \tan \delta_l^r = \frac{\Gamma(E)/2}{(E_r - E)}$$

$$q = -\cot \xi_l(k) \quad = -\frac{1}{\varepsilon} = \frac{b}{a}$$

$$\sigma_l = \frac{4\pi}{k^2} (2l+1) \sin^2 \xi \frac{\left(q - \frac{a}{b} \right)^2}{1 + \left(\frac{a}{b} \right)^2} = \frac{4\pi}{k^2} (2l+1) \sin^2 \xi \frac{(q + \varepsilon)^2}{1 + \varepsilon^2}$$



Fano introduce these parameters which are famously known as Fano's q in epsilon parameters. So, we will introduce this and show the equivalence with the Bright to Wagner formula.

(Refer Slide Time: 33:33)

Configuration interaction in a many-electron system: bound-bound ; bound-continuum

Ugo Fano Physical Review Vol. 124 (1961) p. 1866

'zero' order approximation states of the two-electron system

$$\langle \varphi_d | H | \varphi_d \rangle = E_\varphi$$

$$\langle \psi_{E'} | H | \varphi_d \rangle = V_{E'}$$

$$\langle \psi_{E''} | H | \psi_{E'} \rangle = E' \delta(E'' - E')$$

CI wavefunction: $|\Psi_E\rangle = a_E |\varphi_d\rangle + \int dE' b_{E'}^E |\psi_{E'}\rangle$



And in terms of this we will discuss the autoionization resonances between the bound and mounted continuum transitions.

(Refer Slide Time: 33:44)

Effects of Configuration Interaction on Intensities and Phase Shifts*

U. FANO

$$\varepsilon = -\cot \delta_\ell^{r'}(k)$$

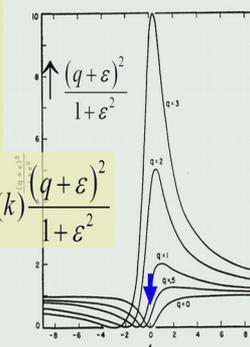
$$q = -\cot \xi_\ell(k)$$

continua and of a set of discrete level intensity shifts produced in a Rydberg section. The interaction with the nucleus

$$\sigma_l = \frac{4\pi}{k^2} (2l+1) \sin^2 \xi_l(k)$$

$$F(E) = P \int dE' \left[\frac{V_{E'}^2}{(E - E')} \right]$$

$$\langle \varphi_d | H | \varphi_d \rangle = E_\varphi$$



ym-
and
stic
ev,
iore
lin-
tra-

FIG. 1. Natural line shapes for different values of q . (Reverse the scale of abscissas for negative q .)

$$E_r = E_\varphi + F(E)$$



So, the shape of a resonance can be just about anything, these are not always symmetric lines across the resonance energy on either side of the resonance energy. You typically have symmetry. So, we will talk about it.

(Refer Slide Time: 34:00)

$\Gamma = 2\pi V_E^2$
 ↑ Resonance width
 $\langle \psi_{E'} | H | \phi_d \rangle = V_{E'}$: determines the resonance width

$\tau \sim \frac{\hbar}{\Gamma}$ ('lifetime' of the autoionization resonance state)

The notion of 'lifetime' is *different* from that of 'time delay' in scattering.

NPTEL
 PCD TACS Unit 1 Select/Special Topics from 'Theory of Atomic Collisions & Spectroscopy' 70

Then we will have, we will introduce the idea of time delay in scattering which is different from that of lifetime of a resonance state. So, you will have the time delay in scattering. (Refer Slide Time: 34:16)

The wave-front appears to have originated from a distance $v_i t \pm \bar{\rho}(\hat{\Omega}) \hat{k}_i$ rather than from $v_i t$.

TIME DELAY $t_d = \frac{\left(\frac{d\delta}{dk}\right)}{v_i}$ derivative of the phase shift with respect to k

$E = \frac{\hbar^2 k^2}{2m} \Rightarrow dk = \frac{m dE}{\hbar^2 k} = \frac{dE}{\hbar v}$

$t_d = \hbar \frac{d\delta}{dE}$

Wigner Eisenbud time-delay
 L. E. Eisenbud, Ph. D. thesis, Princeton Univ. (1948).
 E. P. Wigner, Physical Review 98, 145 (1955).
 F.T.Smith, Physical Review 118:1, 349 (1960)

NPTEL Energy derivative of the phase shift w.r.t. k

PCD TACS Unit 1 Select/Special Topics from 'Theory of Atomic Collisions & Spectroscopy' 71

This is also known as the Wigner Eisenbud time delay because the original formalism was done by Eisenbud and Wigner around 1950 and there are important contributions by Smith and others. So, we will introduce time delay in scattering. (Refer Slide Time: 34:16)



“Wigner Time Delay’
and **‘Resonance life times’**

“Wigner Time Delay’
and **‘Photoionization time-delay’**

PCD TACS Unit 1 Select/Special
Topics from ‘Theory of Atomic
Collisions & Spectroscopy’

72

Which is typically known as the Wigner time delay? And we will relate the Wigner time delays with resonance lifetimes and in the context of the Wigner time delay we will also discuss the time delay in photo emission process or photoionization processes. So, these are the topics that we will cover in this unit.

(Refer Slide Time: 34:57)



Select/Special Topics in Atomic Physics



Unit 8 (3 lectures) Lectures 43 to 46

Three Guest Lectures by
Professor S.T.Manson,
Georgia State University,
Atlanta, USA



PCD TACS Unit 1 Select/Special Topics from ‘Theory of Atomic Collisions & Spectroscopy’ 73

And that will bring us to the guest lectures in the last unit. These guest lectures are delivered by Professor Steve Manson of the Georgia State University and Steve has delivered three lectures.

(Refer Slide Time: 35:12)

Select/Special Topics in Atomic Physics

Unit 8 (3 lectures)

Lectures 43 to 46

- 1) 'Photoionization and Photoelectron Angular Distributions'
- 2) 'Ionization and Excitation of Atoms by Fast Charged Particles'
- 3) 'Photoabsorption by Free and Confined Atoms and Ions: Recent Developments'

These three lectures are on photo ionization of Photoelectron Angular distributions, the lecture two is on Ionization and Excitation of Atoms by Fast Charged Particles and the third lecture is on Photoabsorption by Free and Confined Atoms and he will give you an overview of some other recent developments.

So there will be these three lectures end in the last unit. So, that pretty much sums up an overview of what this course will turn out to be. And I hope that you will benefit from it and the basic idea which I would like to emphasize over here having said that okay it is important to study atomic physics means following the spirit of Feynman Quote that is the most important thing that he would like to leave for posterity.

And how one can really get so much of other knowledge in science by extending atomic physics into other areas then what this course attempts to do is to give you the tools to study atomic physics. So, you need to study atomic physics, atomic structure then atomic dynamics collisions, how an atom is probed using particles or electromagnetic radiation okay.

So, the tools that are necessary, is what I shall attempt to provide in this course. So, thank you very much.

(Refer Slide Time: 36:48)

Select/Special Topics in Atomic Physics

NEXT class:



Quantum Collision Theory – Part 1

STiTACS U1 Lecture number 02

Bye!



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

And we will begin the next lecture with the first lecture of quantum collision physics. Thank you very much.