

Select/Special Topics in ‘Theory of Atomic Collisions and Spectroscopy’
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Lecture 43
Eisenbud formalism of Time-delay in Scattering

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Refer: Previous class; and SITACS, Unit 1, L04, 05, 06

We considered in our previous class –

- how the centre of the scattered wave packet propagates.

C.J. Joachain: Quantum Theory of Collisions Fig. 3.4, p 56

shape of the wave packet

$$\Psi_{\vec{b}}^+(\vec{r}, t) \xrightarrow{r \rightarrow \infty} \Phi_{\vec{b}}(\vec{r}, t) + f(\vec{k}_i, \hat{\Omega}) \frac{e^{i(k_i r - \omega(\vec{k}_i) t)} }{r} e^{-i\vec{k}_i \cdot \vec{b}} \chi(r\hat{k}_i - \vec{v}_i t + \vec{\rho}(\hat{\Omega}) - \vec{b})$$

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Greetings, So, today we have the last class of this unit and also the last class of this course. So, I am pretty much going to wrap up the whole discussion. Let me begin with what we were discussing toward the end of the previous class. We considered the, how the Center of a scattered wave packet progresses after the scattering.

And we considered a wave packet which was not necessarily impacting the target head-on but at a somewhat displaced impact parameter and with reference to this, scattering situation, which we had discussed at considerable length in unit 1 of this course. We wrote the solution to the scattering problem which is very similar to how it looks for a single plane wave.

But this time, this is written up for the entire wave packet. So, you have got a superposition of a good number of mono energetic waves. They may be close to some central momentum.

But there is a little bit of, you know, dispersion.

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$$\Psi_{\vec{b}}^+(\vec{r}, t) \xrightarrow{r \rightarrow \infty} \Phi_{\vec{b}}(\vec{r}, t) + f(\vec{k}_i, \hat{\Omega}) \frac{e^{i(k_i r - \omega(\vec{k}_i)t)}}{r} e^{-i\vec{b} \cdot \hat{\Omega}} \chi(r\hat{k}_i - \vec{v}_i t + \vec{\rho}(\hat{\Omega}) - \vec{b})$$

$$\Psi_{\vec{b}}^{\text{scattered}}(\vec{r}, t) \xrightarrow{r \rightarrow \infty} \frac{1}{r} |f(\vec{k}_i, \hat{\Omega})| e^{i(k_i r - \omega(\vec{k}_i)t + \Lambda(\vec{k}_i, \hat{\Omega}) - \vec{k}_i \cdot \vec{b})} S_f$$

where $S_f = \chi(r\hat{k}_i - \vec{v}_i t + \vec{\rho}(\hat{\Omega}) - \vec{b})$ (shape function)

PHASE ANGLE

$$\Lambda(\vec{k}, \hat{\Omega}) = \Lambda(\vec{k}_i, \hat{\Omega}) + \left[\vec{v}_k \cdot \Lambda(\vec{k}_i, \hat{\Omega}) \right]_{\vec{k} = \vec{k}_i} \cdot (\vec{k} - \vec{k}_i)$$

$$= \Lambda(\vec{k}_i, \hat{\Omega}) + \vec{\rho}(\hat{\Omega}) \cdot (\vec{k} - \vec{k}_i)$$

$$\zeta = k_i r - \omega(\vec{k}_i)t + \Lambda(\vec{k}_i, \hat{\Omega}) + \vec{\rho}(\hat{\Omega}) \cdot (\vec{k} - \vec{k}_i) - \vec{k}_i \cdot \vec{b}$$

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And we looked at the solution for the scattered part alone. So, this is the scattered part which we considered yesterday. We find that the phase, now, depends on a wave vector which is no longer unique; because the wave packet consists of several momenta which are superposed. But they are close by and you can expand them in the neighbourhood of one of them, okay.

The central one like k_i , so, this is the first order expansion that we considered. So, there is this phase angle and then there is a net phase of the scattering amplitude which is the Zeta.

So, Zeta is the net phase of the Scattering Amplitude
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$$\zeta = k_i r - \omega(\vec{k}_i)t + \Lambda(\vec{k}_i, \hat{\Omega}) + \vec{\rho}(\hat{\Omega}) \cdot (\vec{k} - \vec{k}_i) - \vec{k}_i \cdot \vec{b}$$

How would you describe the surface of the scattered wave whose wave front propagates along \hat{k}_i ?

On this surface $\frac{d\zeta}{dk_i} = 0$

$$\frac{d\zeta}{dk_i} = r - \frac{d\omega(\vec{k}_i)}{dk_i} t - \vec{\rho}(\hat{\Omega}) \cdot \hat{k}_i = 0$$

Position of the wavefront: $r(t) = \left[\frac{d\omega(\vec{k}_i)}{dk_i} \right] t + \vec{\rho}(\hat{\Omega}) \cdot \hat{k}_i = v_i t + \vec{\rho}(\hat{\Omega}) \cdot \hat{k}_i$

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And we ask the question how would we describe the surface of a scattered wave whose wavefront propagates along the unit vector \hat{k}_i , okay, which is the unit vector along the central momentum direction. So the criterion would be that on the surface di by dk would be 0. And this leads us by simply taking the derivative of this with respect to k .

A relationship which tells us how the wave-front propagates, ok like a classical object like a classical kinematic relation. And we find that it travels at a group velocity and then it is it seems to have originated from a slightly different point, okay. There is that displacement vector.

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$$f(\vec{k}, \hat{\Omega}) = \left| f(\vec{k}, \hat{\Omega}) \right| e^{i\Lambda(\vec{k}, \hat{\Omega})} \approx \left| f(\vec{k}_i, \hat{\Omega}) \right| e^{i\Lambda(\vec{k}, \hat{\Omega})}$$

$$\vec{\rho}(\hat{\Omega}) = \left[\vec{\nabla}_k \Lambda(\vec{k}_i, \hat{\Omega}) \right]_{\vec{k} = \vec{k}_i} \quad \leftarrow \text{dimension: L}$$

Gradient of the phase of the scattering amplitude with respect to k

$$r(t) = \left[\frac{d\omega(\vec{k}_i)}{dk_i} \right]_{t \pm \vec{\rho}(\hat{\Omega}) \cdot \hat{k}_i} = v_i t \pm \left| \vec{\rho}(\hat{\Omega}) \cdot \hat{k}_i \right| \quad \text{Spatial shift}$$

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

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

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So, essentially the displacement is in terms of the gradient of the phase of the scattering amplitude with respect to k. And the wave-front would appear to have originated because of the phase shift. It would appear as if the wave-front has originated, if there is a delay it from a point behind what you thought is the source.

Or from a point which is ahead of what you believe is the source so from one of the two depending on whether their wave-front has advanced or retarded by this collision process. So, there is a Spatial shift corresponding to which, there is a time delay, ok; because any phase shift corresponds to a time delay or time advancement.

And this time delay would be given by if you if you divide this by the velocity and you get the derivative of the phase shift with respect to k divided by v, which gives you the time delay.

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

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

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

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)

Wigner Eisenbud time-delay

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

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So, this is the result that we obtained which we discussed in our previous class. And we can write this derivative with respect to energy, instead of, with respect to k. And by simply noting that energy goes as k square. And this is the relationship that we get which is famously known as the Wigner Eisenbud time-delay.

It is in terms of the derivative of the phase shift with respect to energy and of course h cross takes care of the dimensions and other proportionality. So, this is the Wigner time delay as we know it.

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δ : phase of the scattering amplitude $f(\vec{k}, \hat{\Omega})$ $\frac{r}{v_i} = t - t_d$

$$t_d = \frac{\left(\frac{d\delta}{dk}\right)}{v_i} \quad \left(\frac{d\delta}{dk} > 0\right) \Rightarrow (t_d > 0) \rightarrow \text{delay}$$

$$\left(\frac{d\delta}{dk} < 0\right) \Rightarrow (t_d < 0) \rightarrow \text{advancement}$$

Long delay in the emergence of the scattered wave means a **sharp increase in the phase δ (greater slope)** as a function of k; $\delta(k)$.

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This is the delta, if in, this is the scattering amplitude. It is a phase of the scattering amplitude. And it is the energy derivative of this or d delta by dk. And you can see from this relation that if d delta by dk is positive, you have a time delay whereas if this is negative you have time advancement, okay.

And the advancement or the delay, the amount of delay or advancement will depend on how rapidly the phase shift changes with k . So, you can certainly expect that in the vicinity of resonance it would change rather rapidly.

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LIMIT on time advancement

$$t_d = \frac{\left(\frac{d\delta}{dk}\right)}{v_i}$$

$\left(\frac{d\delta}{dk} > 0\right) \Rightarrow (t_d > 0) \rightarrow \text{delay}$
 $\left(\frac{d\delta}{dk} < 0\right) \Rightarrow (t_d < 0) \rightarrow \text{advancement}$

$\Delta t_{\text{max}} \approx a/v$

$-a \leq \frac{d\delta}{dk}$

Wigner CAUSALITY condition

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So, yes there can be advancement and the scattered wave could sort of overshoot the wave front of an incoming wave. But it does not mean that you can meet the scattered wave in a detector, even before the incident wave has reached the target at all, okay because there is a certain causality which will limit this.

So, there is a limit on the time advancement and this limit you can get from elementary geometry because you know that the time delay, what are the conditions for time delay in time advancements. In the case of time advancement the time delay would be negative. So, $d\delta/dk$ will be negative. But how negative can it get, okay.

So, if you look at this picture the incident wave is going to interact with the scattering region over a certain width a , and it takes a certain amount of time to cross that, okay. So the maximum time delay or time advancement in this case can at the most be a/v . It cannot be more than that, okay because otherwise causality will be broken.

So, this is the limiting consideration and it puts a limit that $d\delta/dk$ must be greater than or equal to $-a$, because it will be negative because in the case of advancement. But it does not mean that it can keep getting arbitrarily more and more negative; there is a limit to that. And this is known as Wigner Causality condition, okay. It is just based on elementary common sense as most of physics really is.

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δ : phase of the scattering
 amplitude $f(\vec{k}, \hat{\Omega})$

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

TIME DELAY (or advance) during the passage
 of the scattered wave in the interaction region.

L. E. Eisenbud, Ph. D. thesis, Princeton Univ. (1948)
 E. P. Wigner, Physical Review 98, 145 (1955)

- Life time of a resonance.
- Time Delay in Scattering by a Potential.
- Time Delay in Scattering at a RESONANCE state.
- Life time \leftrightarrow Time Delay



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So, here you have phase of the scattering amplitude and you have the time delay or advanced during the passage in the interaction region which is the region over which the scattering takes place. This was worked out Eisenbud PhD theses and then in Wigner's work. And then, Smith has some nice papers on it and there has been a lot of work on it.

But over the years in various domains of Atomic Physics, Nuclear physics and various applications in Collision Quantum, Collision Theory. Now, we have discussed the lifetime of a resonance. We have discussed the time delay in a scattering process by a potential. We can talk about the time delay in scattering at a resonance.

And we can ask, what is the relationship between Lifetime and Time delays, okay? Because all of these are, they have some sort of relationship with each other. They are all on a time scale but what exactly are the relationships I will make a few comments on this, which are quite simple.

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The resonant part of the scattering amplitude in a pure BREIT -WIGNER resonance in the ℓ^{th} partial wave:

From Slide 124 of Unit 6, L39 STITACS:

$$f_{\ell}^r(k, \theta) = \frac{2\ell+1}{k} \frac{\frac{1}{2}\Gamma}{E_r - E - \frac{1}{2}i\Gamma} P_{\ell}(\cos \theta)$$

$$t_d^{r,BW} = \hbar \frac{d}{dE} \left[\arg f^{r,BW}(E) \right] \quad \delta_{\ell}^r = \tan^{-1} \left[\frac{\Gamma(E)}{2(E_r - E)} \right]$$

$$t_d^{r,BW} = \hbar \frac{d\delta_{\ell}^{r,BW}(E)}{dE} = \hbar \frac{d}{dE} \left[\tan^{-1} \frac{\Gamma(E)}{2(E_r - E)} \right]$$

Scattering time delay through a pure BREIT -WIGNER resonance in the ℓ^{th} partial wave:

$$t_d^{r,BW} = \hbar \frac{\frac{1}{2}\Gamma}{(E_r - E)^2 + \left(\frac{1}{2}\Gamma\right)^2}$$

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So, let us look at the resonance itself and I will take the case of the pure Breit-Wigner resonance in the ℓ^{th} partial wave. For this, the partial wave scattering amplitude is given by this expression which we have derived in our earlier classes. And the Breit, this is the Breit-Wigner resonance and the time delay, the Wigner time delay, okay.


Wigner's name keeps coming in Quantum physics everywhere; means okay. He is one of the great contributors to Quantum theory. So, this is the Breit-Wigner Resonance formula. And then, there is a Wigner Time delay, okay. So, this is also Wigner; this t d. And this time delay is then the energy derivative of the argument of this particular scattering amplitude. That is the phase which it will pick up, right.

And it the energy derivative of that phase will give you the Wigner Time delay at the Wigner resonance, at the Breit-Wagner Resonance. So, this is the angle that we have to examine to get this energy derivative. This we have obtained in considerable detail in our previous class, in previous classes set of classes. This angle is given by tan inverse of gamma or twice energy difference where gamma is the resonance width, okay.

So, you remember this relationship. So, you can put this angle over here and that gives you what is the time delay. And this time delay would be h cross energy derivative of this angle. So, this is the energy derivative of this angle which is coming from the scattering amplitude at the resonance and the Breit-Wigner Resonance.

So, this is your net result that your time delay at the Breit Wigner resonance will be given by: if you take the tan inverse of this and take its energy derivative, this is the result that you get. It is a very simple result but also a result which tells us, how to relate the time delay with the lifetimes at a resonance.

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Lifetime of the resonance $\frac{\hbar}{\Gamma} = \tau$

Wigner Time Delay at Resonance $t_d^{r,BW} = \hbar \frac{\frac{1}{2}\Gamma}{(E_r - E)^2 + \left(\frac{1}{2}\Gamma\right)^2}$

Maximum time delay at the resonance $t_{d, \text{MAXIMUM}}^{r, \text{Breit-Wigner}}$ at $E=E_r$ $\left. \vphantom{t_{d, \text{MAXIMUM}}^{r, \text{Breit-Wigner}}} \right] = 2 \frac{\hbar}{\Gamma} = 2\tau$


Maximum Wigner time = twice the life-time of the BW resonance

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So this is the lifetime of the resonance which is just the inverse of the width right and this is the time delay. So, now look at these two expressions and they tell you what the relationship between time delay and life line is. So, the maximum time delay that you can get is obviously at the energy resonance when $E = E_r$. So, this term will go to zero.

And you have got half gamma over its square, right. So, the maximum time delay that you can get at the Breit Wagner resonance will be twice \hbar cross over gamma, or which is twice the lifetime okay. So that is the maximum time delay that you can get at the resonance. So, this is an important result.

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Resonance \leftrightarrow "Quasi - Stationary states"

$E = E_r - \frac{1}{2}i\Gamma$

$\Psi(\vec{r}, t) = \psi(\vec{r})e^{-\frac{E}{\hbar}t} = \psi(\vec{r})e^{-\frac{E_r - \frac{1}{2}i\Gamma}{\hbar}t}$

$= \psi(\vec{r})e^{-\frac{E_r}{\hbar}t} e^{-\frac{1\Gamma}{2\hbar}t}$

$\Psi^*(\vec{r}, t)\Psi(\vec{r}, t) = \psi^*(\vec{r})\psi(\vec{r})e^{-\frac{\Gamma}{\hbar}t}$

probability density diminishes exponentially

Hamiltonian: Non-Hermitian

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And we will, I will pretty much summarize the main points that we have considered in the context of resonances and scattering theory. Resonance then is typically a Quasi-stationary

state. Quasi-stationary state will not have a real energy because it decays, right. And the decay is then contained in an imaginary part of the energy.

So, the decay is then manifest in this expression which is, the width half width is the imaginary part of the complex energy. The Schrodinger wave function is no longer stationary. It is quasi-stationary which means that its probability density will keep diminishing with time. It will not remain invariant with time which is why it is not stationary. And this is the Probability amplitude.

So, if you determine the Probability density, it will diminish exponentially by this function which is determined by the factor gamma, okay. And because the energy is complex you do not get it from a Hermitian, Hamiltonian. So, you can do Quantum mechanics with non Hermitian operators, non Hermitian Hamiltonian; as in Bohm's book on Quantum mechanics is a good source to read about this.

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	Definitions of a Resonance	$f_l^r(k, \theta) = \frac{2l+1}{k} \frac{\frac{1}{2}\Gamma}{E_r - E - \frac{1}{2}i\Gamma} P_l(\cos \theta)$ <small>scattering amplitude</small>
1	$\frac{d\delta_l(E)}{dE}$	Maximum of the energy derivative of the scattering phase shift
2	Quasi-stationary states	$E = E_r - \frac{1}{2}i\Gamma$ $\Psi(\vec{r}, t) = \psi(\vec{r}) e^{-\frac{i}{\hbar}(E_r - \frac{1}{2}\Gamma)t} = \psi(\vec{r}) e^{-\frac{E_r}{\hbar}t} e^{-\frac{\Gamma}{2\hbar}t}$
3	Pole of the scattering amplitude in the COMPLEX ENERGY PLANE at	$E = E_r - \frac{1}{2}i\Gamma$

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So, these are various definitions of resonance that you will come across. You can see it defined in terms of the scattering amplitude or in terms of the energy derivative of the phase shift right, where it changes most rapidly, right. So, that would be one criterion. You can see it described in terms of Quasi-stationary states with complex energies with lifetimes.

Or you can define it as a pole of the scattering amplitude in the complex energy plane. So, in various these are all equivalent ways of defining Wigner resonances and we have dealt with some of these, you know; different shades or different manifestations of the Resonance.

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Energy matrix: $\langle \phi_d | H | \phi_d \rangle = E_\phi$

Discrete state embedded in a continuum **Fano-Feshbach resonance**

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

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

E_2 : metastable state

τ : life-time

Shape resonance

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The resonances we considered are of two kinds: the Fano-Feshbach for which we have a discrete state embedded in a continuum. We also considered the Shape Resonances. (Refer Slide Time: 15:40)

Resonances

below ionization threshold

above threshold

Fano-Feshbach Resonances

CI: bound-bound and bound-continuum configurations.

narrow

Shape Resonances

Decay: one electron escapes to infinity by quantum tunneling through a potential barrier.


broad

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And we observe that the Shape resonances tend to be broad. They are above the threshold. The Fano-Feshbach resonances are relatively narrow. They are below the Ionization thresholds, okay. (Refer Slide Time: 15:54)

- ✓ Interacting atoms
- Unbound (continuum)
- Quasi-bound 'molecular' state



Discrete state
embedded in
a continuum

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Observation of Feshbach resonances in a Bose-Einstein condensate

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These have lots of applications in all domains of Atomic Physics, Nuclear physics, Condensed matter Physics. And in recent years, in the context of Bose-Einstein condensation and getting BEC with Bose mixtures and Fermi mixtures and what not, okay. (Refer Slide Time: 16:19)

- ✓ At low temperatures, the interaction energy of a cloud of atoms is proportional to the (i) density and (ii) a single parameter, the scattering length a .
- ✓ The scattering length *can be modified* by applying external fields: magnetic, optical or rf fields.

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So, what happens is that at low energies scattering is mostly determined by $l = 0$ states by s wave scattering, right. And the single parameter, the scattering length can describe the scattering process. What you can do is control the scattering length by some external fields. It can be a magnetic field; it can be an optical field. And you can control the scattering length and control the scattering mechanism.

So, this is exploited because typically, if you have got Fermi, Fermionic on atoms they will not even get close enough to collide with each other; because of the anti symmetry of the wave function; whereas if you want to cool them, exploiting evaporative cooling, then, you

do need them to interact, okay. So, what you can do is, control this interaction, by modulating the scattering length using some external fields.

And, and that way you can bring about a Bose-Einstein condensation of Fermi atoms, which you would normally think that it is a privilege reserved for the Bose atoms. But then, you can do it with Fermi atoms as well. Because you can have Fermi atoms interact with each other in two kinds of you know, processes.

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Pairing of FERMIONS → BOSONIC states
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

A trapped gas of fermionic ^{40}K atoms
→ 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.

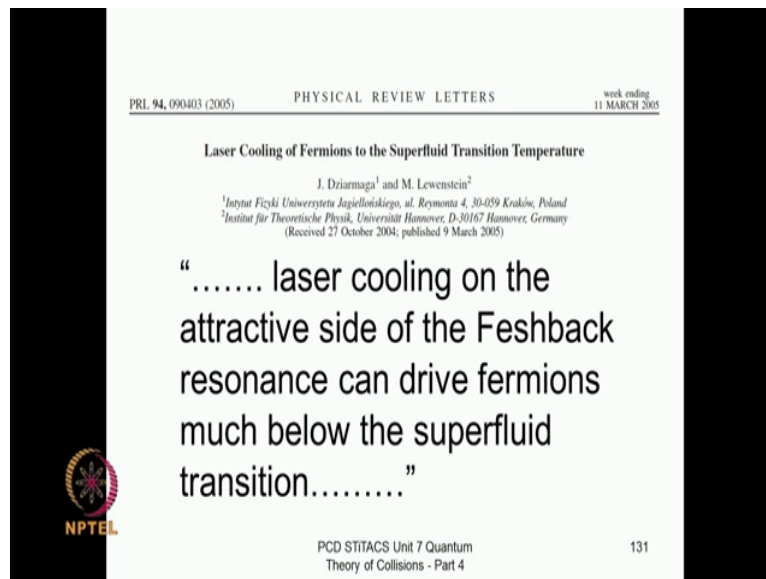
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One is like the unbound state and the other by controlling the scattering length. You can bring them through, swing them through a Feshbach resonance and bring them into a bound state because that's what happens at a Feshbach resonance. You have got the fragments on one side, okay like the atomic case, in which, we had the electron in the continuum.

And the rest of the ion, okay. So, that is those are the fragments that we talked about. Otherwise, you have a doubly excited state in which both the electrons are bound. They are in discrete bound States. So, you have got a bound state and a continuum and the bound state is embedded in the continuum.

So, you can affect a Feshbach resonance and swing them from the fragmented state from the dissociated state, bring them into a bound state and then push them into a condensate. So, that is the technique which is exploited to get BEC with Fermi atoms. And you can do it using magnetic field, induced Fano Feshbach resonances.

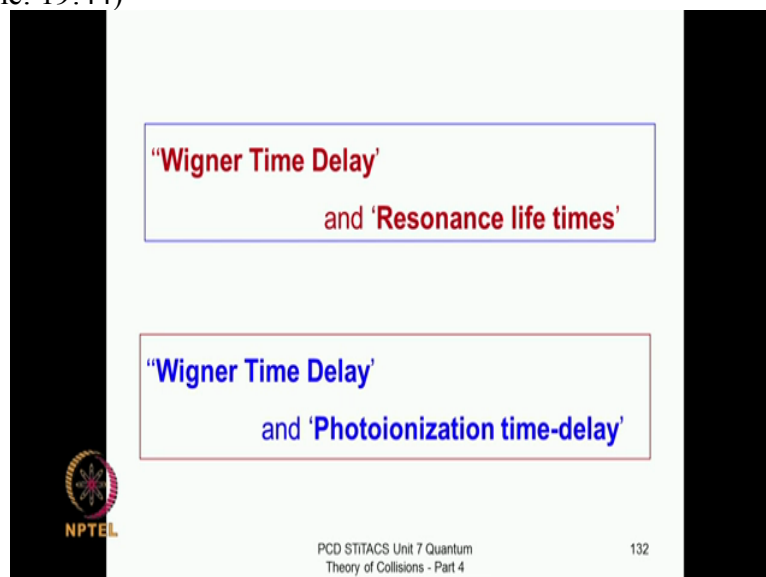
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So, these have large applications in very many different disciplines which are nice things to read. There is a lot of current literature in this area. So, I will hope that some of you will go through the original literature in this area. But the techniques which are fundamental to the understanding of these processes come from Fano's marvellous paper that we have discussed at great length in the last few classes.

So, that paper is really of fundamental importance. So that is the reason that I spend so much time discussing that.

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So, we have discussed, we have discussed the resonance lifetimes; we have discussed Wigner Time delay. And we can also talk about the Photoionization Time- delay; because in photoionization, one always believed that photoionization is an instantaneous process and the electron is kicked out as soon as the electromagnetic energy is absorbed by an atom.

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Reference: Unit 6, STIAP
Special/Select Topics in Atomic Physics

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

collision photoionization

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

Θ : operator for TIME REVERSAL SYMMETRY

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But then, it turns out that there is a little bit of time delay and one can use exactly the same techniques, to study the photoionization time delay. And this relationship comes from what we did way back in actually in the previous course on Atomic Physics in Unit 6 of the special, select topics and Atomic Physics in which we discussed the Time Reversal Symmetry and how it connects.

How it connects the solutions of Collision physics with the solutions of photo ionization. So, we exploit this Time Reversal Symmetry and carry forward the analysis that we learned in scattering theory about the Time delay and use it to determine the Photoionization Time delay.

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Background:

- Quantum Theory of Atoms and Molecules
- Many Electron Theory; HF/DF SCF methods, Many-Body Theories; RPA etc.
- Feynman diagram methods; etc.
- Relativistic Quantum Mechanics

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So, this is when you want to do these calculations in details and I think I am coming toward the end of this course and essentially summing up. You need a good background in the Quantum Theory of Atoms and Molecules. You need a good handle on Quantum Theory of

many electron systems. Hartree Fock and Dirac self consistent fields, Many-body theories, Rhino phase approximation.

You need some capability to address diagrammatic Perturbation theory. And then of course, since Laws of Nature are essentially relativistic there is no escape from Relativistic Mechanics either. So, what we have attempted to do in these courses is to provide an overview of all of these techniques. So, that a graduate student is exposed to these techniques and gets ready, to get into research, in this field.
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STIAP: Special/Select Topics in Atomic Physics 40 Lectures

STITACS: Special/Select Topics in Theory of Atomic Collisions and Spectroscopy 43+3 =46 lectures

Unit 1: Quantum Collisions (L01 – Introduction to STITACS; L02 to L12)

Unit 2: Many-electron Theory (2nd Quantization Methods) (L13 to L15)

Unit 3: Random Phase Approximation (L16 to L24)

Unit 4: Feynman Diagram Methods (L25 to 32)

Unit 5: Collisions (Coulomb scattering, Born Approximation, Quantum Collisions Part 2,3,4 Lippman Schwinger Eq.) (L33 to L35)

Unit 6,7: Resonances (Fano-Feshbach; Life times and Wigner time delay) (L36 to L39; L40 to L43)

Unit 8: Guest Lectures by Prof.S.T. Manson (L44 to L46)

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So, we covered base Atomic Physics in the previous course which is the Select, Special topics in Atomic Physics. And in this course, we have today's as the 43rd lecture. This is the last lecture in this series in unit 7. But then, there are three additional lectures which are given by Professor Manson which are incorporated in this course as Quest lectures.

So, there will be a total of 46 lectures in this course which we covered in these eight units. Today's is the end of the 7th unit. Unit 8 consists of the three guest lectures by Professor Manson and what we have done in unit 1 is given the introduction to Quantum collisions and then we also did quantum Collisions in Unit 5 and Unit 6 and Units 7, which are like part 2 and 3 and 4 of Quantum Collision Theory.

And then, in between, we did the Many Electron Theory, methods of second quantization, Random Phase approximation, Feynman Diagram methods and so on. So, with this, my hope is that we have covered the essential grammar of doing Research in the field of Atomic and Molecular physics.
(Refer Slide Time: 23:44)

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

1. RRPA
2. RRPA-R
3. RMCTD
4. RMQDT

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.

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And with this, you should be able to do, you know, carry out various research applications; handle powerful techniques like the Relativistic Random Phase Approximation, the RPA with relaxation, the Multi configuration, Time tag off Method, the Multi-channel Quantum Defect Theory and so on. So, they are large, you know. There is so much more to learn. And that is far more Advanced Courses or for self-study during your research work. (Refer Slide Time: 24:18)

FAST TRACK COMMUNICATION

Cooper minima: a window on nondipole photoionization at low energy G.B.Pradhan

Ashish Kumar Yadav

Photoionization of Ca 4s in a spherical attractive well potential: dipole, quadrupole and relativistic effects

Ashish Kumar¹, Hari R Varma², Gagan B Pradhan¹, Pranava C Deshmukh^{1*} and Steven T Manson²


Resonance-induced deviations of β from 2.0 for rare gas s-subshell photoionization

S. B. Witfield, R. Wehitz, Hari R. Varma, T. Banerjee, P. C. Deshmukh and S. T. Manson

Hari R Varma Tanima Banerjee 137

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So, many students over here have contributed to, they use these techniques in some applications. There is Gaghan's work and this is not mentioned in any particular order, not chronological order or anything like that, in completely arbitrary order. And some very fascinating applications and Atomic Physics have been studied using the techniques that we have built in these two courses in Atomic Physics. (Refer Slide Time: 24:42)



Photoabsorption studies of some closed-shell ions in the La isonuclear sequence
Sindhu Kalyadan, Hari R. Varma, P.C.Deshmukh, J. T. Costello, P. Hayden and S.T.Manson
Towards a Laser Plasma Light Source Platform for Next Generation Extreme-UV Lithography (EUVL): Theoretical and Experimental Spectroscopic Studies at 6.X nm

Sindhu Kalyaan

PHYSICAL REVIEW A **80**, 023405 (2009)

Nondipole and interchannel-coupling effects in the photodetachment of Cl⁻
J. Jose,¹ G. B. Pradhan,¹ P. C. Deshmukh,^{1,4} V. Radojevic,^{1,2} and S. T. Manson³

Jobin Jose

PHYSICAL REVIEW A **79**, 043401 (2009)


Spin-orbit-interaction activated interchannel coupling in dipole and quadrupole photoionization
S. Sunil Kumar,¹ T. Banerjee,² P. C. Deshmukh,^{1,4} and S. T. Manson³

S. Sunil Kumar

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So, Gaghan, Ashish, Tajima, Sindhu, Jobin and Sunil, lots of students, have contributed to this work.

(Refer Slide Time: 25:03)



Photoionization study of Xe 5s: ionization cross sections and photoelectron angular distributions
G Aarthi^{1,2}, J Jose¹, S Deshmukh¹, V Radojevic¹, P C Deshmukh^{1,4} and S T Manson³

PHYSICAL REVIEW A **89**, 053424 (2014) Aarthi Ganesan

Attosecond time delay in the photoionization of endohedral atoms A@C₆₀: A probe of confinement resonances
P. C. Deshmukh,^{1,2} A. Mandal,¹ S. Saha,¹ A. S. Kheifets,³ V. K. Dolmatov,⁴ and S. T. Manson³

Ankur Mandal

Soumyajit Saha

"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 -"
- Richard Feynman

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And yes, Arthy, Ankur and Soumyajit who are here and I pretty much conclude this course with a quote from Feynman which I love to use repeatedly again and again I am used it in the past. And I like to use it again over here that if in some Cataclysm all scientific knowledge were to be destroyed and only one sentence passed on to the next generation.

Feynman believes it would be the Atomic Hypothesis because he believes that if by studying Atomic Physics, you can use your imagination and get so much more out of it. So, it is really very nice. Atomic Physics is something which I think I absolutely love to learn and to teach because it, it makes use of all the major pillars of physics that uses Classical Mechanics.

It uses Electrodynamics, uses Quantum Mechanics, it uses Statistical Mechanics, Many-body theory. So, all the major powerful pillars of Physics go into this lovely discipline of Atomic Physics.

(Refer Slide Time: 26:21)

Video Courses for NPTEL/NKN Internet Library:

- **Special/Select Topics in Classical Mechanics**
(40 Lectures) – <http://nptel.ac.in/courses/115106068/>
- **Special/Select Topics in Atomic Physics**
(40 Lectures) – <http://nptel.iitm.ac.in/courses/115106057/>
- **Special/Select Topics in Theory of Atomic Collisions & Spectroscopy**
<http://iitmweb.iitm.ac.in/phase2/courses/115106085/>
(46 Lectures) – <http://nptel.iitm.ac.in/courses/115106057/>
- **Video-Seminar on Youtube: An Odyssey in Atomic Physics** <http://www.youtube.com/watch?v=2sP5C7Eh8HY>

NEXT: Unit 8: 3 guest lectures
by Professor S.T. Manson,
Georgia State University, Atlanta

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And here are the web links to the various courses and I must invite you to unit 8 which are three guest lectures by Professor Manson with whom I have had very extensive collaboration over, very many years, for a very long time. And with that I pretty much conclude this.

(Refer Slide Time: 26:46)

Thank you all very much
<https://www.physics.iitm.ac.in/~labs/amp/>

Thanks, of course, to IIT-Madras, NPTEL, NKN

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

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By thanking everybody I have worked with. There are some who are missing in these pictures. It is only illustrative of my gratitude to everybody I have worked with collaborators students. And thanks, of course, to IIT, Madras to the NPTEL staff and team. And thank you all very much for being with me during this course. Thank you.