Selected Topics in Mathematics Physics Prof. V. Balakrishnan Department of Physics Indian Institute of Technology, Madras

Module - 3 Lecture - 8 Linear response; Dispersion relations (Part II)

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In physical practice, what is meant by negative frequency? Just to measure frequencies are all real positive numbers and so on, but there we can use the symmetric property, remember that I could also write this for instance. I could also write this as P over pi integral minus infinity to 0 d omega prime imaginary chi of omega prime over omega prime minus omega plus an integral from 0 to infinity d omega prime imaginary chi of omega prime to minus omega prime.

Then this changes sign, but this becomes infinity to 0 that flips through and I get 0 to infinity, and I get this there is the minus sign here, but imaginary minus omega prime in minus imaginary omega prime, because it was an odd function, so that can this sign here, and you get this plus.

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So, I could not principle write this whole thing as just inside here 1 over omega prime plus omega plus minus, and I add these 2 raise up, and you end up with omega prime square minus omega square, and then a 2 omega prime on top.

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So, it is principle value 2 over pi, this guy goes away mean it, omega prime ((Refer Time: 02:03)) this is equal to the real part. So, now we have find, no matter what omega is for instance a physical positive frequency, it says the real part of the susceptibility at that frequency is the sum or a integral over all other real positive frequencies coming from 0 to

infinity this with this kernel omega prime over omega prime square minus omega square. You could do the same thing for this chi here expect be a minus sign it should appear, and then you get an omega rather than omega prime in the numerator.

So, apart from some sign changes you get an omega here, and you get same denominator. So, we have succeeded and writing expressing for a generalize susceptibility using analyticity which ultimately arouse from causality plus the retarder response and so on. We have succeeded and expressing the real part of this susceptibility as an integral over the imaginary part, and the imaginary part does not integral over the real part. So, these two obey consist they have to obey these relations to be consistent with each other.

It is also clear immediately that neither of them can vanish identically without the other one also vanishing completely, these relations are called dispersion relations. The Hilbert transform relations are called dispersion relations. In physics they are also called Kramer's Kroing relations, because there were originally derived in the context of refractive index, so that is why the word dispersion relation were put in there. So, it related the dispersion coefficient on the dispersion measure of dispersion to the absorption coefficient and vice versa, in this fashion.

Now, all that is gone in here is causality that is the primary thing, the reason for the analyticity was a causality, and causality ensure that you had a Fourier ((Refer Time: 04:32)) transform which made this susceptibility analytic can a certain half plane makes, which half plane it is depended on my Fourier transform convention, had I choosing in the opposite convention had I written function of t as d t d omega into the plus I omega t, it would have been the low half plane which was analytic for the susceptibility that is not important what is crucial is the fact that in one of the 2 half planes you have this analyticity.

We will compute this susceptibility in a little while will computed for some physical system like ((Refer Time: 05: 06)) circuit for example, then you will discover that it explicitly has poles in the lower half plane as it should, because if it were a analytic there to in the whole thing will just be a constant. Now, let us go back and look at one assumption we made here, and see what we can do about that? We it might turn out that this susceptibility does not vanish as the frequency goes to infinity ((Refer Time: 05: 30)) go to some constant for example. Suppose it pardon me

Student: a data function.

May not be however huge variety of cases it may not vanish at all, it may just go to some constant at the end, what would you do? Then this assumption that I made is incorrect, I assume that this big semi circle contribution was 0 that is no wrong at true.

 $V(w) \rightarrow \mathcal{H}_{\infty}(\neq 0) \text{ as } |w| \rightarrow \infty \text{ in the UHP.}$ $\int \frac{dv' \mathcal{H}(w)}{V - v} \quad i \neq 0 \text{ in the UHP.}$ $\int \frac{dv' \mathcal{H}(w)}{V - v} \quad i \neq 0 \text{ in the UHP.}$ V(w) = V(w) = V(w) + v(w) +

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Well, suppose it turns out that chi of omega prime goes to some constant set nor equal to 0 as goes to infinity in the upper half plane. I can do the same calculation as before, but recall what happen? We had not the contribution from this gamma d omega prime chi of omega prime divided by omega prime minus omega. My argument was that when this omega prime was of the form R e to the i theta very large r, when this R and that R canceled each other, and because this went to 0 the contribution from the integral went to 0, but now it is gone to some constant. Well, you can still evaluate it, because that constant is chi infinity, and this R will cancel again this R, and you have an integral from 0 up to pi.

So, you have an extra contribution which should be of the form i pi chi infinity, some constant which you know already. So, it does not affect the dispersion relation should be take decent account you can do this, no difficulty here at all. It is another matter if it does not go to a constant, but goes to a function of omega then you have to worry about it you have to do something else, but even here you have a problem.

Because, I assume that if omega prime goes to 0 along any of these directions in any direction what so ever, this chi went to the same constant chi infinity, there is no reason why that should be the case along different rays it might go to different values might go to different constant, say it is smoothly changes or something like that. Then I cannot do this I cannot do this integral at all, what I then do is a clever treat called subtraction, what you do is you say well I have to pay the price somewhere, I have to know this susceptibility at some point.

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Let us suppose that I know the value of the susceptibility at some point omega naught, I have to know that as input. I do the same thing as before this is omega, this is the omega prime plane, but now I define my function f of omega prime not as chi of omega prime over omega prime minus omega, but rather as chi of omega prime minus chi of omega naught divided by omega prime minus omega naught, I defined it in this fashion. Now, look at what happens to this function here. This is analytic in the upper half plane, it does not go to 0 at infinity, but if it goes to 0 if it goes to a constant or does not raise more rapidly than omega prime itself.

Then this function here still behaves like for very large values of omega prime it still goes to 0 on that semi circle, because now you got a d omega prime with the capital R, that capital R will cancel against this, and as long as this does not go as fast as omega prime, but ((Refer Time: 09:28)) square root of omega prime or some power, this factor will take care of it. So, this will work even if chi of omega prime did not go to 0 in the upper half plane at infinity, but went either going to constant or even groom or exploded it, but not faster than not as fast as omega prime itself this would work. The price you pay is that you have to give me this input information. At some frequency you need to know this, this is called a subtraction point.

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And this is called a subtraction that subtracted dispersion relation, once subtracted dispersion relation.

Student: ((Refer Time: 10:15))

That is right. So, we goes like omega square, omega prime square then I need at least two subtraction I need more and so on. So, I add more points to these, and then keep on adding those guys in the denominator, now clear. So, it is possible as long as it does not blow up like an exponential or something like that which is completely unphysical, it is possible to write subtracted dispersion relations with more inputs you need this at other points.

So, this is proof to be extremely useful this consequence of analyticity, this proof to be extremely useful in practice. For example, in quantum scattering theory written out that if you have scattering of a static potential, the scattering amplitude measures in some sense, the differential cross section measures how much of the incident flux is scattered or some particular angle put a detector, and that measure is calculated from something called the scattering amplitude. The scattering amplitude is a function in potential scattering of the incident energy if it is elastic scattering as well as the scattering angle.

Now, as a function of the momentum transfer between the initial state and the final state as a function of this momentum transfer it turns out that the scattering amplitude satisfies dispersion relations is an analytic. Therefore, you can write down such relationships they are

serve as consistency conditions, and if you know something about this side, on this side you can compute the other portion that is it, in that application this thing is called the absorptive part, and this is the reactive part over error.

But, there a lot sub such applications in physics in quantum field theory to there are cases where scattering amplitudes they would then be relativistic scattering amplitudes would satisfy dispersion relations of this kind, very useful both empirically as well as to test the consistency of a calculations. So, I brought the sub, because we now look at some examples in next time of physical response functions brought the sub to show that this idea of analyticity actually has very deep physically implications as also very direct physical application in case of linear response here in the form of dispersion relations.

There are more such applications, but this is the very primary principle application of the idea of something being analytic. Notice how we went through this, we assumed that this function existed for real omega, and then I simply said there is an analytic continuation I looked at this integral. So that shows that definite integrals can be used to define analytic continuations, and we will develop that the little further, earlier I gave a method of analytic continuation by looking at series by writing down power series, but here I did not do that I just had a definite integral, and then I argued that this definite integral itself gives you a representation of an analytic function.

I will use the gamma function as an example to show how that I get can be developed to write down an analytic continuation. This susceptibility in general in linear response is defined as the Fourier lap transform form of some response function, and it is an analytic function in the upper half plane in the frequency in our notation in our convention, and it satisfies dispersion relations whereby the real and imaginary parts forms a Hilbert transform pair. Now, just to give you feel for very specific example let us taken an extremely simple case very standard example the damped simple Harmon gauss latter or in the electrical analogy the LCR circuit.

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And a typical LCR circuit with the voltage attached to it is going to look like the differential equation is this, so LCR series circuit these plus R times I plus the capacitance part that is the charge. So, it is 1 over C an integral from minus infinity to t d t prime I of t prime that is the total charge accumulated in the capacitor until time t, this is equal to your applied voltage V of t in the standard notation. So, you have an inductance, resistance, and the capacitance, and there are series, so that is equal to the applied voltage on the right hand side.

Now, you could ask what is the susceptibility of the system, in other words given a voltage what is the response like the current response like, and I do the usual Fourier transforms, and it is clear that since I write I of t as d omega e to the minus I omega t etc, when I differentiate with respect to t I am pulling down a factor of minus I omega. On the other hand when I integrate I am pulling down I am dividing by a factor of minus I omega. So, it is clear we can immediately write down this going to be minus I omega L plus R plus 1 over minus i omega C on I tilde of omega, this is v tilde of omega it follows immediately that this is so.

Therefore, I write I tiled of omega equal to in the standard notation is to write it in terms of an admittance here a sudden Y, so Y of omega times V tilde of omega where this quantity is reciprocal of these guys. So, let us do the following let us write this is minus, and write it in this form, and multiply through by I omega. So, this by tilde of omega is going to be an i omega divided by this i omega multiplies and gives me omega square, I take out L plus R over l i omega minus 1 over L C which is the standard admittance for an LCR circuit. (Refer Slide Time: 16:52)

So, rewriting this we therefore have Y of omega equal to i omega divided by L times that is the inertia term omega square plus i gamma omega minus omega naught square. So, if we recall the undammed L C circuit has a natural frequency omega naught equal to 1 over square root of L C, and the time constant of this thing is gamma inverse where gamma is R over L. So, the L R circuit has a time constant which is L over R, and the L C circuit has natural frequency 1 over square root of L C. So, in terms of those two quantities this is the susceptibility if you like.

Now, this obviously has poles in the denominator, and the question is where are these poles? It cannot be in the upper half pane, they cannot be in the upper half plane. So, these poles are going to be at poles simple poles at omega equal to minus i gamma over 2 plus or minus square root of where thus minus gamma square, and then 4 here plus omega naught square. So, let us look at the under damped case, and this is going to become then omega naught square square, I took out the 4 in order to divide the 2 out, so this is going to be minus gamma square over 4 under damped.

As you know under damping is when omega naught is less then gamma over 2, and over damping is when omega this is the under damped case when omega naught is bigger than gamma over 2, and the over damped case will be when the sign is flipped in the critically damped cases when omega naught is exactly gamma over 2. Now, where are these poles located? Well, if it is under damped omega naught this implies omega naught square is

greater than gamma square over 4. So, these poles are going to be at in the omega plane, it is minus I gamma over 2.

So, immediately you see that it is going to have negative imaginary part and then plus or minus certain things, so it is 1 pole it is going to sit here another pole is going to sit here in the omega plane. As long as there is it is resistance the dissipation in other words this gamma is a positive number, if you did not had that if you had negative feedback then of course, you can have a runaway solution if you have a wrong sign of the friction constant then off course you have a solution which blows up on the other hand for physical circuits for physical resistances as we have used a convention the same convention as before, the poles are in the lower half plane.

So, this tells you that certainly you can expect a generalize susceptibility to have one or more singularities in the lower half plane always, whenever there is some dissipation in the system this is always going to be the case, by the way what is going to happen to it when it gets critically damped over damped etc. what is going to happen to these poles? Where are they going to go?

Student: critical damp.

This fact that they are in the lower half plane cannot change that cannot change at all. So, what will happen? Then omega naught becomes exactly equal to gamma over 2 is this appears, and the 2 poles coincide.

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So, these 2 guys move like this, move like this they coincide, and after that what happened next? If I go to the over damped case what is going to happen?

Student: ((Refer Time: 20:49))

But, they comes at time when this positive sign and this negative sign will cancel out, and give you 0, so what will happen is this fellow will crawl up in this fashion, and this guy will crawl down in this fashion, and go off to minus infinity. So, as you change the friction for instance keeping a fixed omega naught this is are the 2 poles are going to wander around, but the fact is they will always remain in the lower half plane ((Refer Time: 21:17)) that is required by causality. There has to be an electricity in the upper half plain, and so no matter what you do this is all that is going to happen in circuit.

This is exactly the simple damped simple harmonic cause later, for which you recall that L is replaced for instance by the mass, this by the friction, the viscosity of a medium in which the particle moves. And that thing gives you the natural frequencies, the restoring force of the undammed oscillator. The lots and lots of other analogies many, many second order equal systems, would have exactly the same sort of dynamics here. So, this portion plus that portion these two terms together, these guys give you the reactive part of the response, and this gives the deceptive part this case.

So, it is not hard to see now, that this Y of omega will satisfy those relation that I mention,

namely the imaginary part is going to have anti symmetric behavior. And there is real part is going to have symmetric behavior you can check that out. In fact as in exercise you should do the following, you should show that the real and imaginary parts of this Y for real frequencies, satisfy those dispersion relations I mentioned. In this case you can do that fairly easily, because you actually have an explicit answer for the susceptibility itself, so it should be straight forward to do that. Now what can we say in general, well in physics what happens? In physical applications, what happens is something fairly intricate depending on the system.

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The simplest model you can think of, for this response function by the way the susceptibility was given, if you recall by d t it will be e i omega t phi of t. And the simplest thing you can think of for this phi of t, this response function is that it dies down exponentially with some characteristic relaxation time. Lots of media do that and that is called a relaxation time, the characteristic time with which this decay is exponentially. So, for instance a phi of t could be equal to some constant e to the minus t over tau, where this guy this tau is called the relaxation time, what happens then?

So, lot of physical systems and the first approximation would behave in this fashion with one characteristic relaxation time, what happens then? This problem can be solve completely, because you can now write down what this put this phi of t in here, and compute what this thing does. And then chi of omega is equal to well if I put e to the minus t over tau, and I do

this integral e to the minus a t is just 1 over a for positive a or if it is a real part of a is positive which it is in this case, because tau is positive. And you get phi naught divided by 1 over tau, so there is a tau over 1 minus i is in i omega tau, so that is it.

This is an extremely simple form further susceptibility, let us separate it in to real and imaginary parts, I write this as 1 plus on top. And then it becomes phi naught tau times 1 over 1 plus omega square tau square plus i omega over 1 plus square tau square. So, as promised the real part is symmetric in omega, the imaginary part is odd and odd function of omega, exactly as we had seen on general grounds. So, this sort of thing is called Debye relaxation, this is the characteristic single relaxation time.

They detail mechanism of where is tau comes from, what is the dissipation inside the medium and so on depends on the problem, but Debye first wrote this form down this implies the approximation, for instance dielectric relaxation for dielectrics this is the exactly how things would behave. And elastic relaxation in mechanical, in mechanical behavior of metals for instance would behave exactly the same way etcetera, etcetera. So, huge number of phenomena are model by this kind of thing this susceptibility, what do they do next well, empirically you know that the standard thing to do is to plot the real part of the susceptibility versus the imaginary part by eliminating the frequency, and that is got a lot of names.

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It had most common name for it is called Cole - Cole plot. This plots if you like the real part of chi versus the imaginary part of kai. In other words you treat chi of omega as a complex variable, and write down where it is for different values of omega, and so called argent diagram, and what is it going to look like here? This is the real part, and that is the imaginary part. Well start with 0 frequency, then the imaginary part is get 0, the real part is 1 in units of phi naught tau. So, let us divide through by this divided by this constant phi naught tau is just given by this.

So, the real part is at unity it is at 1 here, and the imaginary part is 0, and that is it omega equal to 0, and what happens as omega tends to infinity? This course like a 1 over omega dies down, this course like a 1 over omega square, so it dies down extremely sharply, and in fact as you will know these 2 form part of a semicircle it looks like this, this is this point is omega equal to 0, this point is omega tends to infinity, and it is a semicircle centered about the point a half.

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I leave you to verify it is very trivial verification to show that real kai, let us call real chi equal to u, imaginary chi equal to v I leave you to show that u minus a half whole square plus v square equal to 1 4th half square. So, what is done experimentally is to measure the dissipation, measure the reactive part and the dispersion, and then plot one against the other as a function of frequency, and fit a curve of this kind to it. If it exactly fits a semicircle namely this is a 90 degree thing, and that is a 90 degree thing remember experimentally you can only do a few frequencies.

So, you extrapolate or interpolate between the experimental points, and if you can fit a

semicircle to it, then the deduction is that your relaxation process took place with 1 single relaxation time. This is the famous Debye relaxation formula. On the other hand, experimentally what is found is very often departures from this relaxation from this behavior.

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Most often what happens is that the curve looks like this. So, it is an arc of a circle, and it does not intersect at 90 degrees, and is not a semi circle in this case. And then there are other complicated shapes that you can have deformation of this etcetera, etcetera. What primary conclusion would you come to as soon as you see that the shape is not a semi circle?

Student: more parameters.

You need more parameters, more specifically you need more relaxation times that this system does not have a single characteristic relaxation time, but has the whole spectrum of relaxation times, and then all sorts of complicated things can happen.

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For example, suppose it turned out that phi of t. So, if it turned out that phi of t was equal to some lower and upper cut between some lower and upper cut offs. So, let us call this tau min, tau max, and then a whole spectrum d tau e to the minus t over tau with some spectral functions sigma of tau some weight factor out here. And then a whole lot of super pose position of relaxation times continues super position in this case. Then you got a lot of parameters to play with you got this you got that, you got that function and so on. And now if you put it in then each of these times is going to give me a behavior like 1 over whatever it is.

So, for instance real chi is going to look like integral tau min, tau max d tau sigma of tau over 1 plus omega square tau square. Now, it is a predict complicated function of frequency, because you have to do this integral first, and what you get is your function of frequency it is still symmetric in omega, and the imaginary part will have an omega on top, and integrate the same thing, but now all kinds of behavior are possible, very complex behavior is possible.

If you have just a set of discreet relaxation times just a few of them countable, and a finite number, then the formula is just a sum of Debye like terms usual single relaxation times is relatively easy to analyze, but this kind of thing is more characteristic of what actually happens in the system. So, this is a game which you can play depending on the substance, depending on the experiment, depending on the physical problem that we are looking at fairly complicated relaxation phenomena can occur.

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Now, this is a microscopic approach to attend the sense that is not entirely phenomenal logical, what people would do here is should try to modify empirically they try to modify the Debye form for instance, they ride a thing like not 1 over 1 minus i omega tau, but 1 minus omega tau to sum for alpha, and then the whole thing to sum for beta, and so on all search of parameterization use completely empirically.

But, this is a more physical approach to it, because it says you must tell me something about the microscopic mechanics, and then I compute what this a spectrum of relaxation times is and so on. Little later if the opportunity present itself, we will go back and I will show that depending on what you measure and what you what the hamlet what the energy of the system is how it is pump energy is pumped into the system.

This phi of t you can write in explicit formula for it in terms of the physical observables pertaining to a system, and characteristically it is some ensemble average, if you keep your system in thermal equilibrium deviate from it a little bit by applying the external force, then it is typically a correlation time, a finite temperature correlation time classically or quantum mechanically and you can actually compute what it is under suitable approximation. I will do that a little later if time permits we will solve a problem with a spectrum on the in this fashion.