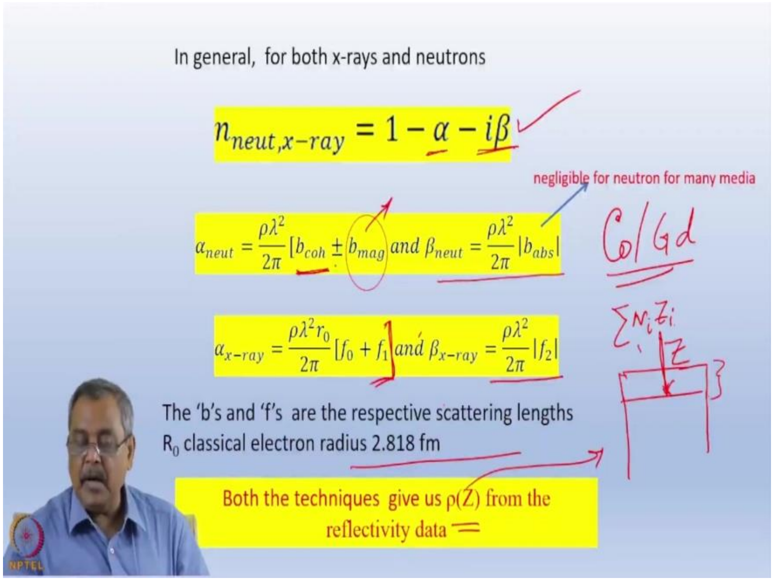
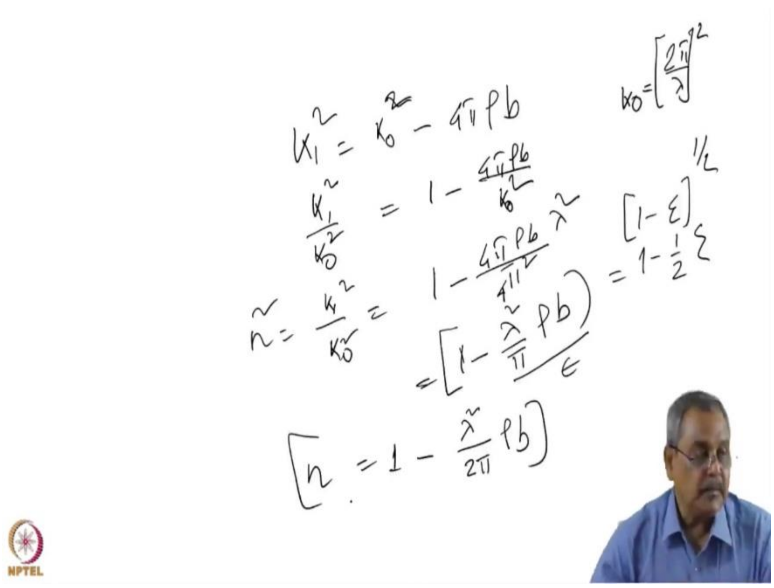
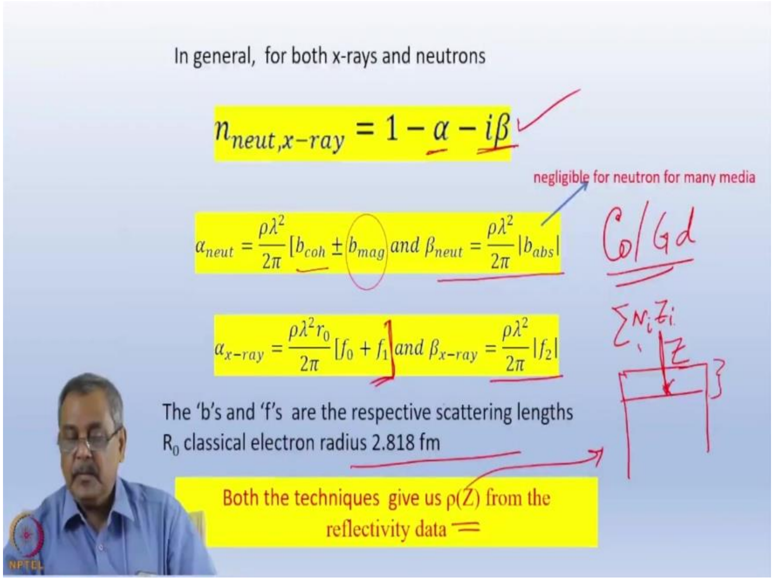
Neutron Scattering for Condensed Matter Studies
Professor Saibal Basu
Department of Physics
Homi Bhabha National Institute
Week 8: Lecture 21C

Keywords: Reflectometry, Critical angle, Scattering length density, Reflected intensity

(Refer Slide Time: 00:13)







Before I go on to the next module, allow me to correct a small mistake that I made. I found that

$$k_1^2 = k_0^2 \ - 4\pi b\rho$$

From this,

$$n = \frac{k_1}{k_0} = \left(1 \ - \frac{4\pi b\rho}{k_0^2}\right)^{1/2}$$

As $k_0 = 2\pi/\lambda$, so,

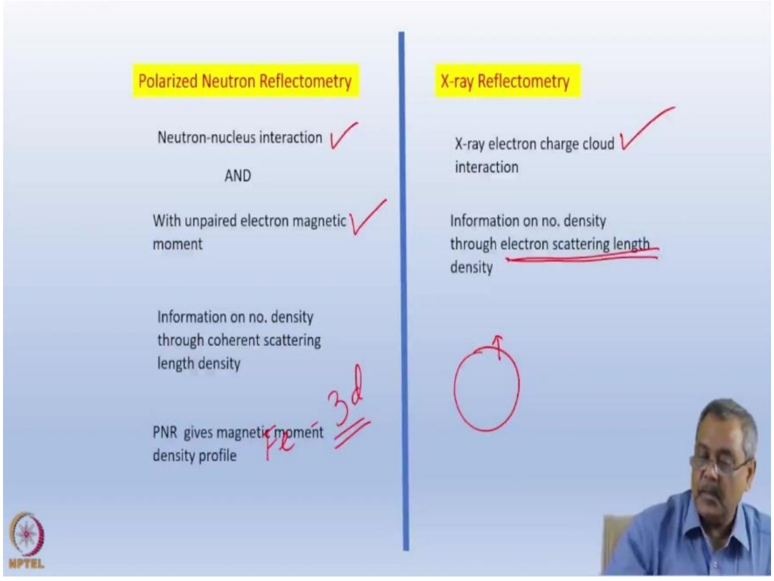
$$n = \frac{k_1}{k_0} = \left(1 - \frac{\lambda^2 b\rho}{\pi}\right)^{1/2}$$

Assuming, $\frac{\lambda^2 b\rho}{\pi} \ll 1$,

$$n = 1 - \frac{\lambda^2 b\rho}{2\pi}$$

This is what I obtain assuming the k changes as the neutron travels in the medium. I also showed you that the refractive index in case of x-rays depends on electron density while in case of neutrons, let me emphasize, it depends on coherent scattering length density and for a magnetized medium, it also depends on magnetic scattering length, which is added or subtracted to the nuclear part depending on whether the medium is polarized and whether the neutron polarization is parallel to it or anti-parallel to it.

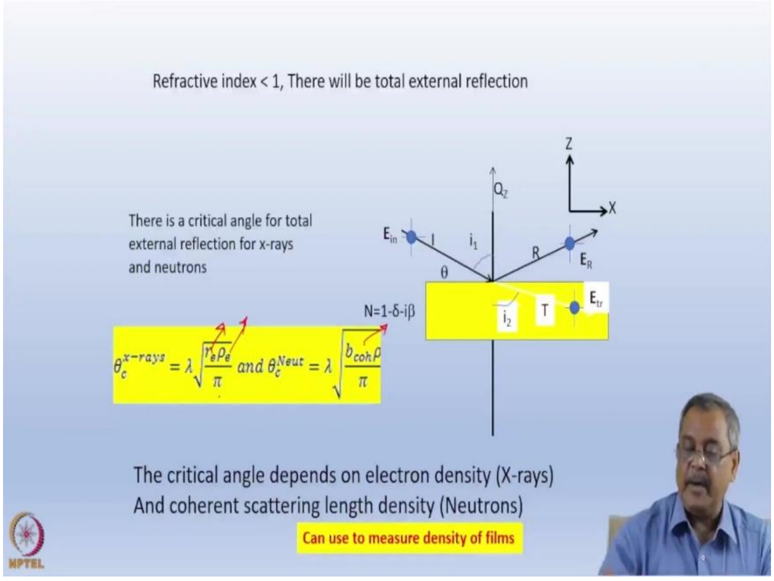
(Refer Slide Time: 03:28)

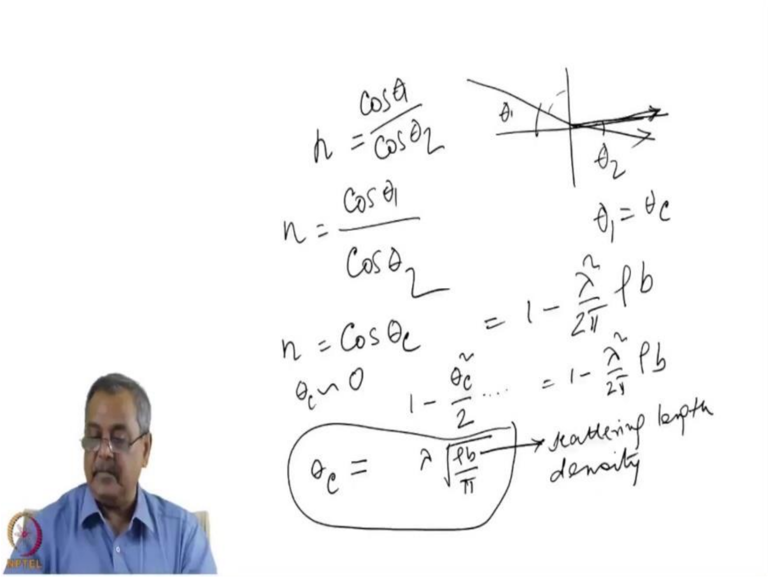


Now, I quickly summarize polarized neutron and x-ray neutron reflectometry. As I told you they are complementary techniques and it depends on neutron-nucleus interaction in case of unpolarized neutron reflectometry and for polarized neutron reflectometry also on interaction with unpaired electron moments giving rise to magnetic moment. To understand this, take a simple example a 3d group magnetic material, say Fe. Every iron atom has got an unfilled shell *'d'* giving rise to its magnetic moment. In this case, the neutron can interact with the nucleus (b_{coh}) and it also interacts with the unpaired electron's magnetic moment. Hence, we get information on number density through coherent scattering length density and also on magnetic moment density from polarized neutron reflectometry.

In case of x-ray reflectometry, it is x-ray and the electron charge cloud interaction and information on electron density is obtained through electron scattering length density. That means, on the same sample, I can use coherent scattering length density in case of neutron reflectometry and use electrons scattering length density in case of x-ray reflectometry. I can translate these densities physical density. There is a unique technique that using these two techniques together, I can actually obtain the density of a two-component medium from the above considerations. So, this was a quick comparison between polarized neutron reflectometry and X-ray reflectometry.

(Refer Slide Time: 05:29)





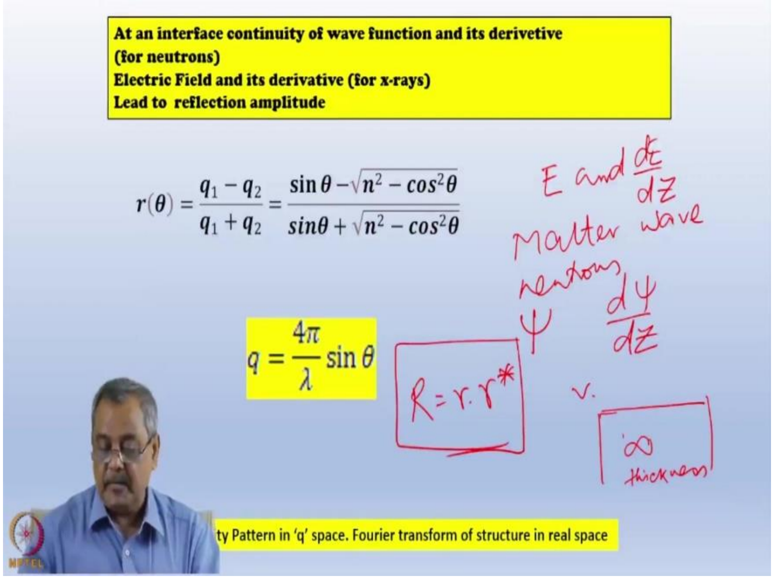
Now, let me just try to figure out what should be the reflectivity of a medium and what should be the critical angle for a medium that I discussed earlier. I want to show you that for specular reflectometry, there is an incident beam, there is the reflected beam and there is a transmitted beam in the medium. Because the medium has refractive index < 1 so there is possibility of total external reflection and the I will just derive the critical angle for reflection. for you.

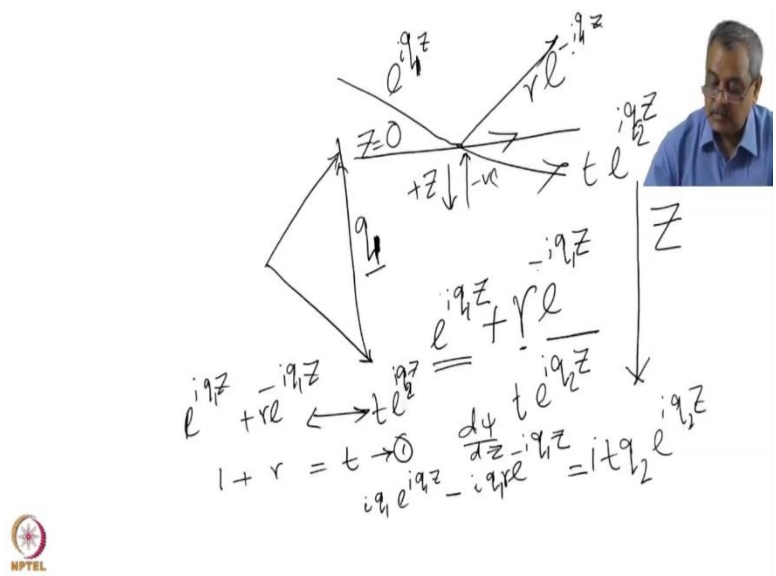
For a material, if incident beam makes an angle θ_1 with the surface of the material, while the refractive beam makes and angle θ_2, in this refractive index is given by, $n = \frac{\cos\theta_1}{\cos\theta_2}$. If I have measured the angles from surface normal then it would have been, $n = \frac{\sin\theta_1}{\sin\theta_2}$. Now, if θ_1 is equal to critical angle then θ_2 becomes 0, the beam starts propagating exactly along the interface. In this case, θ_1 is the critical angle, θ_c and $n = \cos\theta_c = 1 - \frac{\lambda^2 b\rho}{2\pi}$.

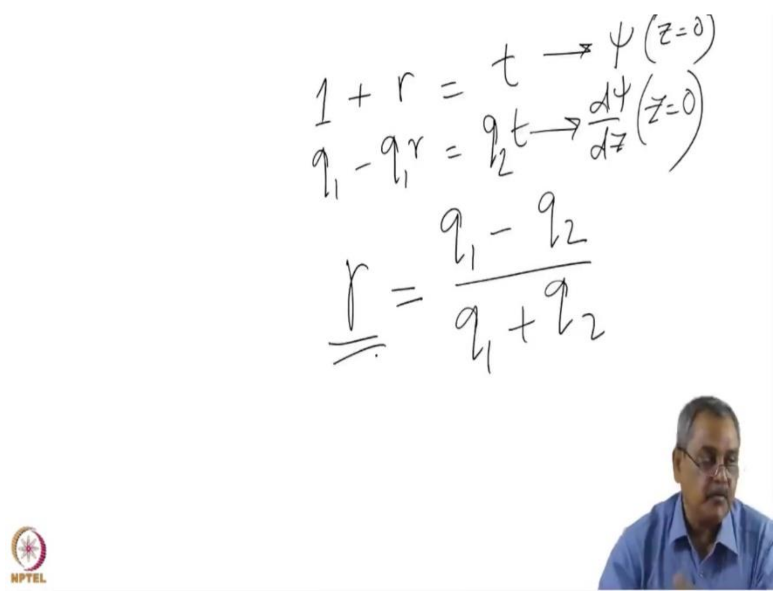
Under the assumption that θ_c is almost equal to 0, we can write $\cos\theta_c = 1 - \frac{{\theta_c}^2}{2\pi}$, so that, $\theta_c = \lambda\sqrt{\frac{\rho b}{\pi}}$. Hence, please note that the critical angle is decided by the scattering length density of the medium. Now, this answers our question that how we can find out density of a medium by measurement of deflection angle. So, one method is the measurement of the critical angle θ_c.

In a similar way, critical angle for x-rays can be written as, $\theta_c^{x-rays} = \lambda\sqrt{\frac{r_e\rho_e}{\pi}}$ where $r_e$is classical electron radius and ρ_e electron density. So, the critical angle in case of x-rays depends on electron density while on coherent scattering length density in case of neutrons. Remember that, so far in this expression I have not added magnetism, where $b = b_{coh} \pm b_m$.

(Refer Slide Time: 09:41)







Now, how do I evaluate the reflectivity at an interface?

In case of x-rays, the electric field (E) and $dE/_{dz}$ should be continuous at the interface. In case of matter wave, like neutrons, it should be the the wave function ψ and its derivative $\frac{d\psi}{dz}$, which should be continuous at the interface Let me just show you. I am talking about an interface in which specular reflection is taking place. Assume the unit amplitude incident wave, $e^{iq_1 z}$ and if r is a reflectivity coefficient and t is transmission coefficient then we have we have got $re^{-iq_1 z}$ in air (vacuum) as the reflected beam and $te^{iq_2 z}$ as the transmitted beam. In this discussion, I have only z-component, an one dimensional problem. Why this is so? Let me explain it to you.

This is the incident beam and the reflected beam I shifted here. This is the q in the medium and same thing is true for the scattered beam. Now, I call it q_1 which is in vacuum. In case of reflectometry, in Snell's law the in-plane components (x and y) they remain unchanged. The only component of wave vector which is changing is the z-component. I am calling it q_1 here and q_2 in the medium and I am considering the propagation is only in z-direction and there is only vector which is changing from one medium to another.

So, now I have got incident beam plus reflected beam, $e^{iq_1 z} + re^{-iq_1 z}$. Exponents have different signs for incident and reflected beam because if incident beam is taken in +z-direction then reflected beam is in -z-direction. This is only for the z-component and I am not bothered about x, y components. The incident beam is of unit amplitude while r is reflection amplitude. The transmitted beam amplitude is $te^{iq_2 z}$.

From the continuity of wavefunction across interface, we have

$$e^{iq_1 z} + re^{-iq_1 z} = te^{iq_2 z}$$

Putting z=0, we have, $1 + r = t$.

Similarly, from the continuity of $d\psi/dz$ we have,

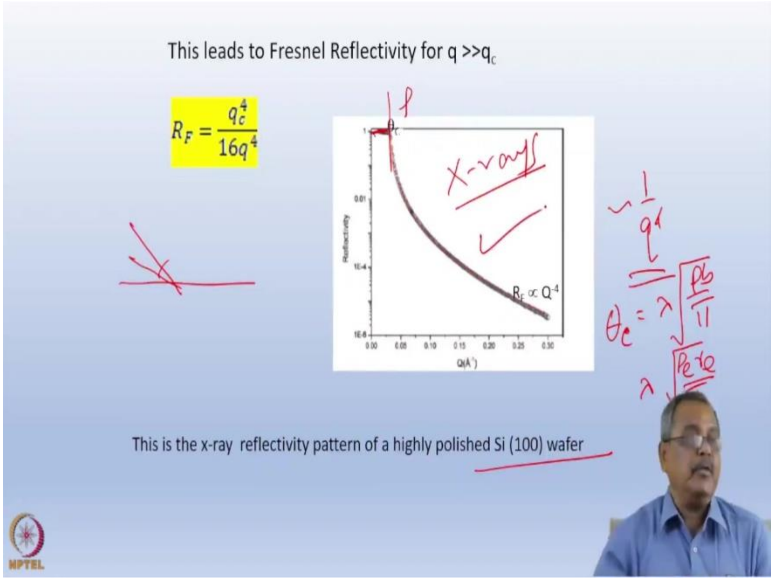
$$iq_1 e^{iq_1 z} - iq_1 re^{-iq_1 z} = iq_2 te^{iq_2 z}$$

Putting z=0, we have, $q_1(1 - r) = q_2 t$

If I solve these two equations, then we get, reflection amplitude, $r = \frac{q_1 - q_2}{q_1 + q_2}$.

If we use the expression, $q = \frac{4\pi}{\lambda}\sin\theta$ then we can get the expression for r in terms of sins and cosines. From this, reflected intensity is given by, $R = r.r^*$. This is the reflected intensity for an interface between vacuum and a medium of infinite thickness. The reflectivity pattern that I will get in q space is Fourier transform of structure in real space. Basically, I will be studying reflectivity as a function of angle if it is a reactor source, or as a function of wavelength as well as angle if it is a spallation neutron source. We will be probing the reflected intensity in the q space and.

(Refer Slide Time: 17:36)



I just show you the experimental reflectometry result for a highly polished silica surface. This is how it looks like. As I showed you earlier that up to a critical angle the reflected intensity is one and beyond that the reflected intensity falls and when q is very large (>> q$_c$), it falls as $1/q^4$. I will come to it later. So, reflectivity is 1 up to a certain critical angle and falls rapidly at large q. The critical angle is a signature of the density of the medium as the critical angle is given by $\lambda\sqrt{\frac{r_e\rho_e}{\pi}}$ in case of x-rays and $\lambda\sqrt{\frac{\rho b}{\pi}}$ in case of neutrons. So, x-rays will give me the electron density. If I measure it with neutrons, it will give me scattering length density. In the shown case it is x-rays and this tells you what is the density of the medium from which we get this reflectivity pattern. With this I will stop today. I will carry on in the next lecture with discussions on reflectometry.