

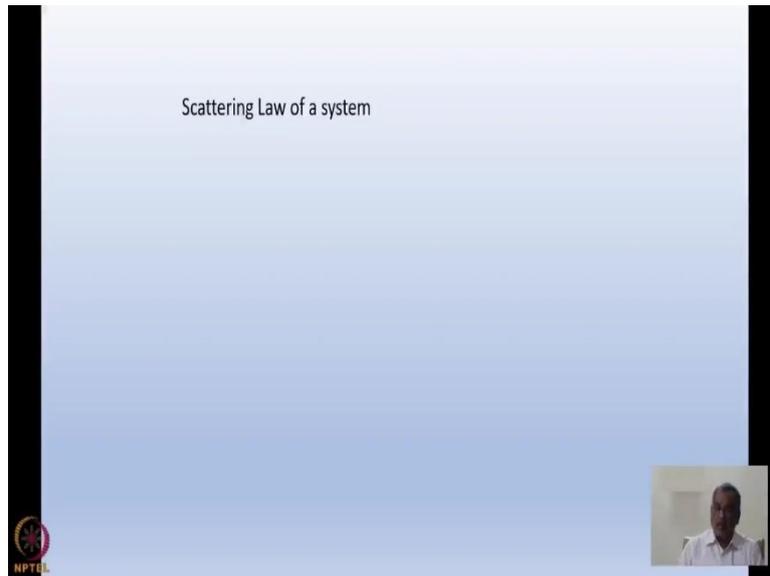
Neutron Scattering for Condensed Matter Studies
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Week 02
Lecture 05A

Keywords: Correlation function, Fourier transform, real space, momentum space

In previous lectures, we have derived the scattering amplitude for lattice at 0 K and at finite temperature. Then we introduced the energy conservation through a δ -function and derived the time correlation, which is correlated to the double differential scattering cross section for a scattering system.

Now, I will introduce you to the correlation functions in real space and time (r,t) to Q,ω -space. It is important as in our experimental results sometimes we will be talking about the real space and sometimes we may talk about Q space and the correlations. Planning of the experiments sometimes will also depend on this.

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$$\frac{d^2\sigma}{d\Omega dE'} = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt e^{-i\omega t} \sum_{jj'} \overline{V_j^+(Q) V_{j'}(Q)} \times \sum_{\lambda} \exp(-\beta E_{\lambda}) / Z$$

$$\times \left\langle \lambda \left| \sum_{jj'} e^{-iQ \cdot R_j(0)} e^{iQ \cdot R_{j'}(t)} \right| \lambda \right\rangle$$

If I take away the site dependence of the potential

$$\frac{d^2\sigma}{d\Omega dE'} = \left(N \frac{K'}{K} \left(\frac{m}{2\pi\hbar} \right)^2 \overline{V^2(Q)} S(Q, \omega) \right)$$

$S(Q, \omega)$ is known as the scattering law for the system

We had derived the scattering law of a system. By scattering law what I mean is that $\frac{d^2\sigma}{d\Omega dE'}$ is a Fourier transform of sum over jj' $V_j V_{j'}$ and then there is a statistical average and sum over all possible sites (distinct as well as non-distinct over ensemble average where we have used the statistical average).

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt e^{-i\omega t} \sum_{jj'} \overline{V_j^+(Q) V_{j'}(Q)}$$

$$\times \sum_{\lambda} \exp(-\beta E_{\lambda}) / Z \left\langle \lambda \left| \sum_{jj'} e^{-iQ \cdot R_j(0)} e^{-iQ \cdot R_{j'}(t)} \right| \lambda \right\rangle$$

Now, other assumption is if I take away the site dependence of the potential means if the potential at all the sites is same, then this part I can take out of the summation and multiply it by N and the factor K'/K is here because of the flux normalization. And I can write as average of $V^2(Q)$.

$$\frac{d^2\sigma}{d\Omega dE'} = N \frac{K'}{K} \left(\frac{m}{2\pi\hbar} \right)^2 \overline{V^2(Q)} S(Q, \omega)$$

$S(Q, \omega)$ is known as the scattering law of the system.

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So, writing $\frac{d^2\sigma}{d\Omega dE'}$ it comes out as $\overline{V^2(Q)}$ and a summation. When you take site dependent average value of that of the potential it comes out of the summation series as it is averaged over that and also we have got $\sum_{jj'} e^{-iQ \cdot [R_j(0) - R_{j'}(t)]}$.

In the expression of differential scattering cross section, time correlation function is averaged over all the possible values of energy with a statistical weightage given by $p_\lambda = \exp(-\beta E_\lambda) / Z$, here $\beta = 1/kT$ and Z is the partition function.

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$$\frac{d^2\sigma}{d\Omega dE'} = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt e^{-i\omega t} \sum_{jj'} \overline{V_j^+(Q) V_{j'}(Q)} \times \sum_{\lambda} \exp(-\beta E_{\lambda}) / Z$$

$$\left\langle \lambda \left| \sum_{jj'} e^{-iQ \cdot R_j(0)} e^{iQ \cdot R_{j'}(t)} \right| \lambda \right\rangle$$

If I take away the site dependence of the potential

$$\frac{d^2\sigma}{d\Omega dE'} = \left(\frac{N K^T}{K} \frac{m^2}{2\pi\hbar} \overline{V(Q)^2} S(Q, \omega) \right)$$

$S(Q, \omega)$ is known as the scattering law for the system

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$$S(Q, \omega) = \frac{1}{2\pi\hbar N} \int_0^\infty dt \exp(-i\omega t) \sum_{jj'} \langle \exp(-iQ \cdot \hat{R}_j(0)) \exp(iQ \cdot \hat{R}_{j'}(t)) \rangle$$

Statistical average Correlationat time t

Define a Fourier transform over 'Q' for the correlation <.....>, a Green's function G(r,t)

$$G(r, t) = \left(\frac{1}{2\pi}\right)^3 \int d^3 Q e^{-iQ \cdot r} \frac{1}{N} \sum_{jj'} \langle \exp(-iQ \cdot \hat{R}_j(0)) \exp(iQ \cdot \hat{R}_{j'}(t)) \rangle$$

Expression for S(Q, ω) is,

$$S(Q, \omega) = \frac{1}{2\pi\hbar N} \int_0^\infty dt e^{-i\omega t} \sum_{jj'} \langle e^{-iQ \cdot \hat{R}_j(0)} e^{-iQ \cdot \hat{R}_{j'}(t)} \rangle$$

which is $\frac{1}{2\pi\hbar N}$ multiplied by the Fourier transform over this statistical average of correlation function at time t. This is actually Q dependent and we take away the time dependence over a time Fourier transform, we get that Q and ω dependence. Similarly, we can go to r-space from Q-space using a Fourier transform as below,

$$G(r, t) = \left(\frac{1}{2\pi}\right)^3 \int d^3 Q e^{-iQ \cdot r} \frac{1}{N} \sum_{jj'} \langle e^{-iQ \cdot \hat{R}_j(0)} e^{-iQ \cdot \hat{R}_{j'}(t)} \rangle$$

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$$G(r, t) = \int d^3Q \sum_{ll'} \langle l | e^{iQ \cdot r} | l' \rangle I(Q, t)$$

Here, I performed the integration over Q space. I have to do a Fourier transformation over Q now, that means, if there is function I(Q,t) in momentum and time space and I perform a Fourier transformation over Q then we go to real space and time, G(r,t).

Similarly, if one does a Fourier transformation over time (t) then we are in omega space and vice versa. This is an interesting way of looking at our data, we collect our data in S(Q, ω) in terms of scattering law of a system.

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$$Q = \frac{4\pi}{\lambda} \sin \theta$$
$$I(Q) \rightarrow G(v)I$$
$$I(Q, \omega) \leftarrow I(Q, t) \leftarrow G(v, t)$$

For example, for a diffraction experiment, we know $Q = \frac{4\pi \sin \theta}{\lambda}$, this is momentum transfer and we know that we collect the intensity as a function of Q . We will get this kind of Bragg peaks. So, we get intensity as a function of Q .

From here, if we want to go to the real space then we need to do a Fourier transform and we get correlation functions in r -space, $G(r)$. For inelastic experiments, if I am in real space, $G(r, t)$, one Fourier transform will take me to Q and time space, $I(Q, t)$, and one more Fourier transform will take me to Q and energy transfer (ω) space, $I(Q, \omega)$. These are the correlation functions in Q, ω -space, Q, t -space, and $G(r, t)$ is the physical system whose expression we are seeking.

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$$S(Q, \omega) = \frac{1}{2\pi\hbar N} \int_0^{\infty} dt \exp(-i\omega t) \sum_{jj'} \langle \exp(-iQ \cdot \hat{R}_j(0)) \exp(iQ \cdot \hat{R}_{j'}(t)) \rangle$$

Statistical average Correlationat time t

Define a Fourier transform over 'Q' for the correlation <.....>, a Green's function G(r,t)

$$G(r, t) = \left(\frac{1}{2\pi}\right)^3 \int d^3 Q e^{-iQ \cdot r} \frac{1}{N} \sum_{jj'} \langle \exp(-iQ \cdot \hat{R}_j(0)) \exp(iQ \cdot \hat{R}_{j'}(t)) \rangle$$

This is known as a Green's function when you go to real space and time, which is a Fourier transform over Q; $\int d^3 Q e^{-iQ \cdot r} I(Q, t)$ of the correlation function summed over all the sites,

$$G(r, t) = \left(\frac{1}{2\pi}\right)^3 \int d^3 Q e^{-iQ \cdot r} \frac{1}{N} \sum_{jj'} \langle e^{-iQ \cdot \hat{R}_j(0)} e^{-iQ \cdot \hat{R}_{j'}(t)} \rangle$$

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Prescription from real space (r) and time (t) to Q, ω space: energy and momentum transfer

$$S(Q, \omega) = \frac{1}{2\pi\hbar N} \int_{-\infty}^{+\infty} dt e^{-i\omega t} \int d^3 r e^{iQ \cdot r} G(r, t)$$

Now, the prescription for real space (r) and time (t) to Q, ω-space is the Fourier transform over energy and momentum. Hence, S(Q, ω) is a double Fourier transform of G(r,t).

$$S(Q, \omega) = \frac{1}{2\pi\hbar N} \int dt e^{-i\omega t} \int d^3 r e^{iQ \cdot r} G(r, t)$$

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$$S(Q, \omega) = \int dt \int d^3r e^{i\vec{Q} \cdot \vec{r}} G(r, t)$$


Here, one Fourier transform is over space (r) and another Fourier transform over time (t).

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One more: the intermediate scattering function

$$I(Q, t) = \int d^3r e^{i\vec{Q} \cdot \vec{r}} G(r, t)$$

This gives

$$S(Q, \omega) = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} dt e^{-i\omega t} I(Q, t)$$

FT on time/energy FT on space/momentum

$$S(Q, \omega) \longleftrightarrow I(Q, t) \longleftrightarrow G(r, t)$$


There are many ways to talk about a diffraction. I can do it by setting $\omega = 0$ then it will be $S(Q)$ and I can also do it as an integration over ω . These two I will take up the next part of my lecture.