Lec 16: shah, function

Set-up

1) X-ray: Are they waves?
If so, then the wavelength $\approx 10^{-8}$ centimeter. too small to observe

2) Crystals: macroscopic structure is somehow determined by the atomic structure,
atoms arrayed on a lattice
how to test that

Study the atomic structure of crystals via diffraction experiments with X-rays

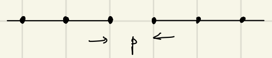
Hypothesis:

1). X-rays are waves, will diffract
(diffraction depends on the size of aperture relative to the wave length)

2). crystals have a lattice atomic structure.
the spacing of the atoms is comparable to the wave length of X-ray

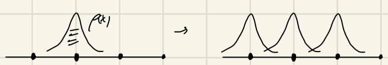
· One - dimension picture

think of the one-dimensional crystal as an array of evenly spaced atoms alone a line



(infinite line)

want to study the electron density distribution for the crystal
the electron density distribution for the crystal is a peridized version of that of a single atom
$\rho(x)$ is the density around a single atom
the density for the crystal is $\rho_p(x) = \sum_{k=-\infty}^{+\infty} \rho(x-kp)$



diffraction determined by the F.T of $\sum_{k=-\infty}^{+\infty} \rho(x-kp)$

· Shah function

Write $\rho_p(x)$ as a convolution

$$\rho(x-kp) = \rho(x) * \delta(x-kp)$$

$$(f*g)(x) = \int_{-\infty}^{+\infty} f(u)\, g(x-u)\, du$$

$$\rho(x-kp) = \int_{-\infty}^{+\infty} \rho(u) \cdot \delta(x-kp-u)\, du$$

$$\tau_{kp}\, \rho = \rho * \tau_{kp}\, \delta$$

$$\rho_p(x) = \sum_{k=-\infty}^{+\infty} \rho(x-kp)$$
$$= \sum_{k=-\infty}^{+\infty} \rho(x) * \delta(x-kp)$$
$$= \rho(x) * \left(\sum_{k=-\infty}^{+\infty} \delta(x-kp)\right)$$

Shah function (of spacing p): $Ш_p(x) = \sum_{-\infty}^{+\infty} \delta(x-kp)$

$\rho_p(x) = \rho(x) * Ш_p(x)$

$\mathcal{F}\rho_p = (\mathcal{F}\rho)(\mathcal{F}Ш_p)$ want $\mathcal{F}Ш_p$

does $Ш_p$ make sense as a distribution

take $p=1$ $Ш(x) = \sum_{k=-\infty}^{+\infty} \delta(x-k)$

$Ш$ makes sense as a distribution

$\langle Ш, \phi \rangle = \sum_{k=-\infty}^{+\infty} \langle \delta(x-k), \phi \rangle = \sum_{k=-\infty}^{+\infty} \phi(k)$ will converge when ϕ is a rapidly decreasing function

$\langle \mathcal{F}Ш, \phi \rangle = \langle Ш, \mathcal{F}\phi \rangle = \sum_{k=-\infty}^{+\infty} (\mathcal{F}\phi)(k)$

could write $(\mathcal{F}Ш)(s) = \sum_{k=-\infty}^{+\infty} (\mathcal{F}\delta)(s) = \sum_{k=-\infty}^{+\infty} e^{2\pi iks}$, but this doesn't converge classically, but it's ok as a distribution

Poisson summation formula:

if ϕ is a rapidly decreasing function, then $\sum_{k=-\infty}^{+\infty} \phi(k) = \sum_{k=-\infty}^{+\infty} (\mathcal{F}\phi)(k)$

ϕ is a given rapidly decreasing function. periodize ϕ to have period 1

$\Phi(x) = \sum_{k=-\infty}^{+\infty} \phi(x-k)$

$$\begin{aligned}\hat{\Phi}(n) &= \int_0^1 \Phi(t)\, e^{-2\pi int}\, dt \\ &= \int_0^1 \sum_{k=-\infty}^{+\infty} \phi(t-k) \cdot e^{-2\pi int}\, dt \\ &= \sum_{k=-\infty}^{+\infty} \int_0^1 \phi(t-k) \cdot e^{-2\pi int}\, dt \qquad u = t-k \\ &= \sum_{k=-\infty}^{+\infty} \int_{-k}^{-k+1} \phi(u) \cdot e^{-2\pi in(u+k)}\, du \\ &= \sum_{k=-\infty}^{+\infty} e^{-2\pi ink} \cdot \int_{-k}^{-k+1} \phi(u)\, e^{-2\pi inu}\, du \\ &= \sum_{k=-\infty}^{+\infty} \int_{-k}^{-k+1} \phi(u)\, e^{-2\pi inu}\, du \\ &= \int_{-\infty}^{+\infty} \phi(u)\, e^{-2\pi inu}\, du = (\mathcal{F}\phi)(n)\end{aligned}$$

expand Φ in F.S

$$\begin{aligned}\Phi(x) &= \sum_{k=-\infty}^{+\infty} \hat{\Phi}(k)\, e^{2\pi ikx} \\ &= \sum_{k=-\infty}^{+\infty} (\mathcal{F}\phi)(k)\, e^{2\pi ikx}\end{aligned}$$

$$\begin{cases} \Phi(x) = \sum_{k=-\infty}^{+\infty} \phi(x-k) \\ \Phi(x) = \sum_{k=-\infty}^{+\infty} (\mathcal{F}\phi)(k)\, e^{2\pi ikx} \end{cases}$$

evaluate at $x=0$

$$\sum_{k=-\infty}^{+\infty} \phi(k) = \sum_{k=-\infty}^{+\infty} (\mathcal{F}\phi)(k)$$

$$\begin{aligned}\langle \mathcal{F}Ш, \phi \rangle = \langle Ш, \mathcal{F}\phi \rangle &= \sum_{k=-\infty}^{+\infty} (\mathcal{F}\phi)(k) \\ &= \sum_{k=-\infty}^{+\infty} \phi(k) = \langle Ш, \phi \rangle\end{aligned}$$

$\mathcal{F}Ш = Ш$

$$Ш_p(x) = \sum_{k=-\infty}^{+\infty} \delta(x-kp)$$
$$= \sum_{k=-\infty}^{+\infty} \delta\left(p\left(\frac{x}{p}-k\right)\right)$$
$$= \frac{1}{p} \sum_{k=-\infty}^{+\infty} \delta\left(\frac{x}{p}-k\right)$$
$$= 1/p\ Ш(x/p)$$

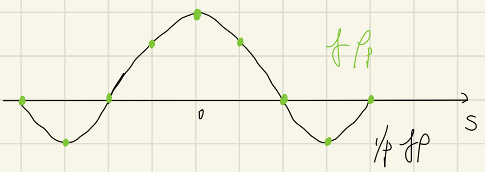
$$(\mathcal{F}Ш_p)(s) = \frac{1}{p} \mathcal{F}(Ш(x/p))(s)$$
$$= \frac{1}{p} p \cdot (\mathcal{F}Ш)(ps) = Ш(ps)$$
$$= \sum_{k=-\infty}^{+\infty} \delta(ps-k) = \frac{1}{p} \sum_{k=-\infty}^{+\infty} \delta\left(s-\frac{k}{p}\right)$$
$$= 1/p\ Ш_{1/p}(s)$$

$\mathcal{F}Ш_p = 1/p \cdot Ш_{1/p}$ (reciprocal relationship !)

· Crystals

$$\rho_p = \rho * Ш_p$$
$$(\mathcal{F}\rho_p)(s) = (\mathcal{F}\rho)(s) \cdot (\mathcal{F}Ш_p)(s)$$
$$= (\mathcal{F}\rho)(s) \cdot 1/p \cdot Ш_{1/p}(s)$$
$$= 1/p\ (\mathcal{F}\rho)(s) \sum_{k=-\infty}^{+\infty} (\tau_{k/p}\delta)(s)$$
$$= 1/p \sum_{k=-\infty}^{+\infty} (\mathcal{F}\rho)(s)(\tau_{k/p}\delta)(s)$$

$$\mathcal{F}\rho_p = 1/p \cdot \sum_{k=-\infty}^{+\infty} \underbrace{\mathcal{F}\rho}_{\text{intensity}} \cdot \underbrace{\tau_{k/p}\delta}_{\text{impulse, only 1 at } x = nk/p}$$



Spacing of the diffraction spot is proportional to the reciprocal of spacing of atoms