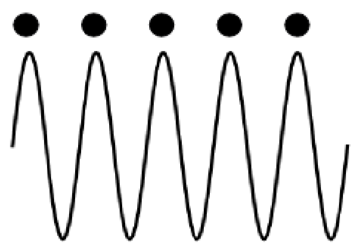
Topic 3-0: Fourier Series
Kittel Pages: 27,28

Summary: Here Fourier series are introduced as a way to build complicated periodic functions from other periodic functions that are easier to work with. We first use sines and cosines to build functions and then introduce using complex exponentials instead. Complex exponentials will be used in Fourier series in this class for the rest of the semester.

- At 0 K, any local crystal property, like position of nuclei or charge density, is invariant under the translation vector $\vec{T}$
    - $n(\vec{r}+\vec{T})=n(\vec{r})$
- Start with a one dimensional chain of atoms



- The dots represent atoms in the chain, the wave at the bottom represents the charge density, n(x)
- Since n(x) is periodic we can build it from a sum of periodic functions, like sines and cosines
- Must use a Fourier series

$$n(x) = n_0 + \sum_{p>0} c_p \cos\left(\frac{2\pi p x}{a}\right) + s_p \sin\left(\frac{2\pi p x}{a}\right) \qquad [1]$$

    - In this case c_p and s_p are Fourier coefficients, p is an integer, a is the lattice constant
- Since we are summing over only integer values of p this makes our Fourier space a set of discrete points where these points are associated with waves that satisfy the required translational symmetry of the lattice
- Let's test the requirement of translational symmetry: replace x with $x+a$ in the Fourier series expression and see if we get the original expression back

$$n(x+a) = n_0 + \sum_{p>0} c_p \cos\left(\frac{2\pi p(x+a)}{a}\right) + s_p \sin\left(\frac{2\pi p(x+a)}{a}\right) \qquad [2]$$

- Separating out the addition term in the numerator of the sum we get

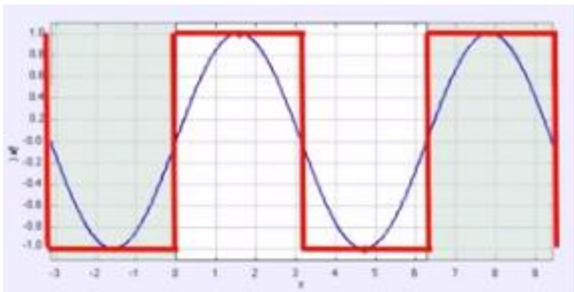
$$n_0 + \sum_{p>0} c_p \cos\left(\frac{2\pi px}{a} + 2\pi p\right) + s_p \sin\left(\frac{2\pi px}{a} + 2\pi p\right) \quad [3]$$

- Since cos(x+2π)=cos(x) and sin(x+2π)=sin(x) this gives us back our original expression for *n*(*x*)

- The Fourier coefficients (c_p, s_p) tell us a particular wave's contribution to the whole n(x)
  - Can also use a complex exponential instead of sines and cosines in a Fourier series. *We will use complex exponentials for the rest of the semester*
  - Complex exponential form:

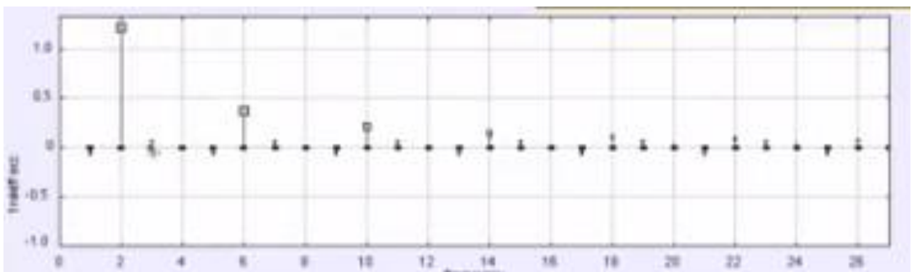
$$n(x) = \sum_p n_p e^{\frac{i2\pi px}{a}} \quad [4]$$

  - In this case the coefficients can be complex and the sum is taken over all values of integer *p*
  - To ensure n(x) is real we must constrain our coefficients
- Fourier series are a way to construct complicated periodic function from a sum of periodic functions that are easy to work with
- When using a Fourier series be sure to use enough terms in the sum that the coefficients decay away and the graph is a good approximation of the function shape desired



- The above is an example of a bad fit
  - The blue line is the Fourier series approximation of the red square wave

- The above is an example of a good fit
  - The blue Fourier series approximation of the red square wave oscillates closely about the desired function
  - It can be seen below that the Fourier coefficients decay away which indicates that we are using enough terms in our sum



Questions to Ponder

1. We discussed the Fourier series in 1D ($n(x) = \sum_p n_p e^{\frac{i2\pi px}{a}}$). How would you extend this sum to 3D?

2. Where is this Fourier space? Consider units to help formulate a response.

3. Does changing the basis change which points in Fourier space are allowed?