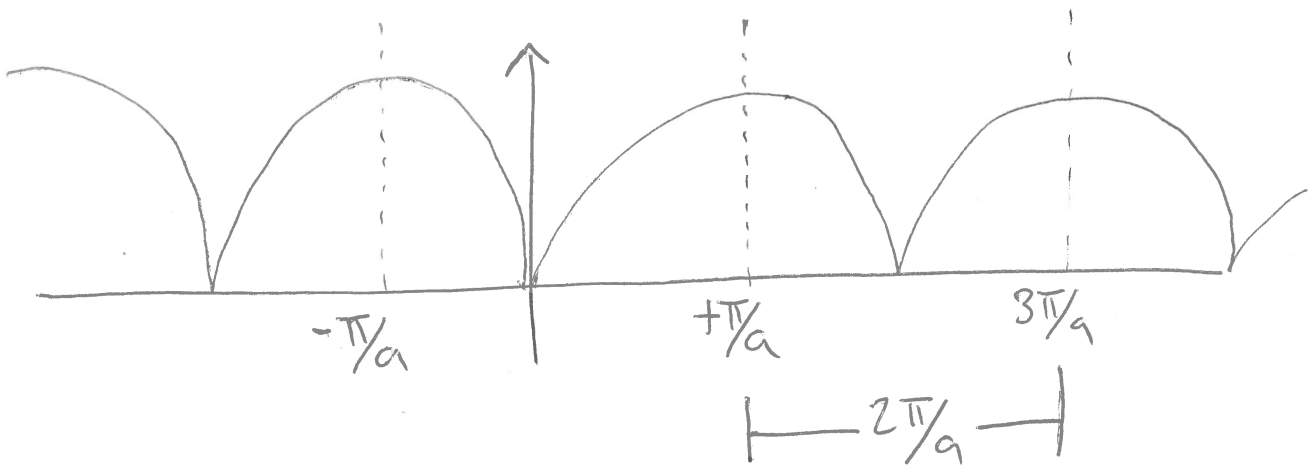
Fri. Oct. 19

- let's review our first encounter with k-space
- a 1D lattice is defined by points $R = na$ where n = integer
- for this solid, we found a dispersion relation $\omega = \omega_{max} \left| \sin\left(\frac{ka}{2}\right) \right|$



- we see k-space or reciprocal space is periodic along k-axis, with periodicity $2\pi/a$
- to generalize if $x \rightarrow x + a$

  then $k \rightarrow k + 2\pi/a$

- recall the unit cell in k-space is the Brillouin zone

- as a quick check

$$U_n = Ae^{i\omega t - ikna}$$

$$k \to k + 2\pi/a \Rightarrow U_n = Ae^{i\omega t} e^{-i(k + 2\pi/a)na}$$

$$= Ae^{i\omega t} e^{-ikna} \underbrace{e^{-i2\pi n}}_{1}$$

$$= U_n$$

- thus k is periodic just as x is.

- clearly shifting k to $k + 2\pi p/a$ for any p = integer, gives us k back

- for $k = 0$, we see equivalent points at locations $\pm 2\pi p/a$

- these points, periodic in k-space, make up the reciprocal lattice

$\longrightarrow$

real: $x_n = \ldots -2a, -a, 0, a, 2a, \ldots$

recip: $G_n = \ldots -2\left(\frac{2\pi}{a}\right), -\frac{2\pi}{a}, 0, \frac{2\pi}{a}, 2\left(\frac{2\pi}{a}\right), \ldots$

- the connection between the two lattice types is given by

$$e^{i G_m x_n} = 1$$

where m, n = integers

- in other words, G_m is only a reciprocal lattice member if eq. above is true

- in general (3D case) we have

$$e^{i \vec{G} \cdot \vec{R}} = 1$$

where $\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$

$\vec{G} = m_1 \vec{b}_1 + m_2 \vec{b}_2 + m_3 \vec{b}_3$

for $\vec{b}_1, \vec{b}_2, \vec{b}_3$ being primitive lattice vectors

- in order for $e^{i\vec{G}\cdot\vec{R}} = 1$, we find

$$\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij}, \quad \delta_{ij} = \begin{cases} 1, & i=j \\ 0, & i\neq j \end{cases}$$

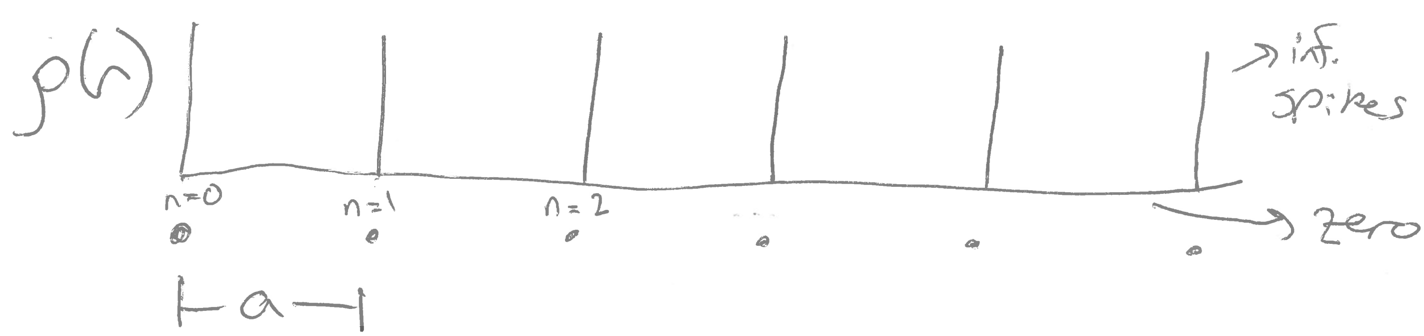
- let's define the density of a real lattice (where points are & are not)

$$\rho(r) = \sum_n \delta(r - an)$$

(assuming periodic b.c.'s)

$$\boxed{\delta(r) = \begin{cases} \infty, & r=0 \\ 0, & \text{else} \end{cases}}$$

where δ is the Dirac delta function



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- let's take the Fourier transform

$$\mathcal{F}[\rho(r)] = \int e^{ikr}\rho(r)\,dr$$

$$= \sum_n \int dr\, e^{ikr}\,\delta(r-an)$$

$$\int \delta(x)\,dx = 1$$

- recall in 1D $\int \delta(x) f(x)\,dx = f(0)$

or $\int \delta(x-a) f(x)\,dx = f(a)$

- so $\sum_n \int dr\, e^{ikr}\,\delta(r-an) = \sum_n e^{ikan}$

$$= \frac{2\pi}{|a|}\sum_m \delta(k - 2\pi m/a)$$ "resummation formula" (non-trivial)

- check: $e^{ikan} = e^{ian[2\pi m/a]} = e^{i2\pi mn} = 1$ for $n, m =$ integers

or $k = 2\pi m/a$ is in the reciprocal lattice

- the take-home message is the following:
  the reciprocal lattice is the Fourier transform of the real lattice

- We note that there is nothing stopping us from performing the same operation for any periodic function $\rho(\vec{r}) = \rho(\vec{r}+\vec{R})$, for $\vec{R} \equiv$ lattice vector

$$\mathcal{F}[\rho(\vec{r})] = \int d\vec{r}\, e^{i\vec{k}\cdot\vec{r}} \rho(\vec{r})$$

- We will come back to the details of this soon, but the answer we get is

$$\mathcal{F}[\rho(\vec{r})] = (2\pi)^D \sum_{\vec{G}} \delta^D(\vec{k}-\vec{G}) S(\vec{k})$$

$$S(\vec{k}) = \int d\vec{x}\, e^{i\vec{k}\cdot\vec{x}} \rho(\vec{x})$$

- structure factor $\rightarrow$ how material scatters radiation