Playing with waves

The theory of diffraction

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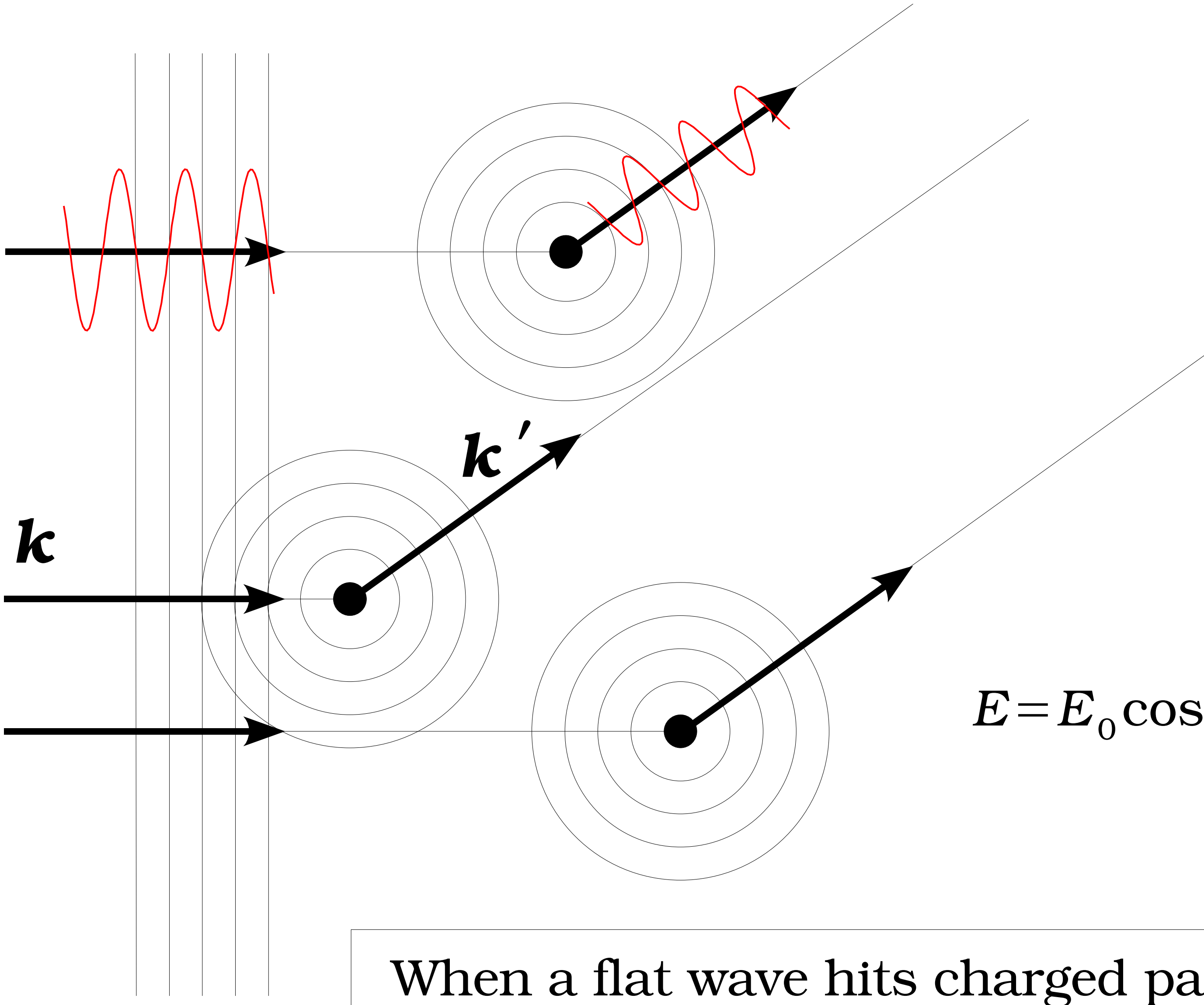
2007

Scattering of waves (X-rays)



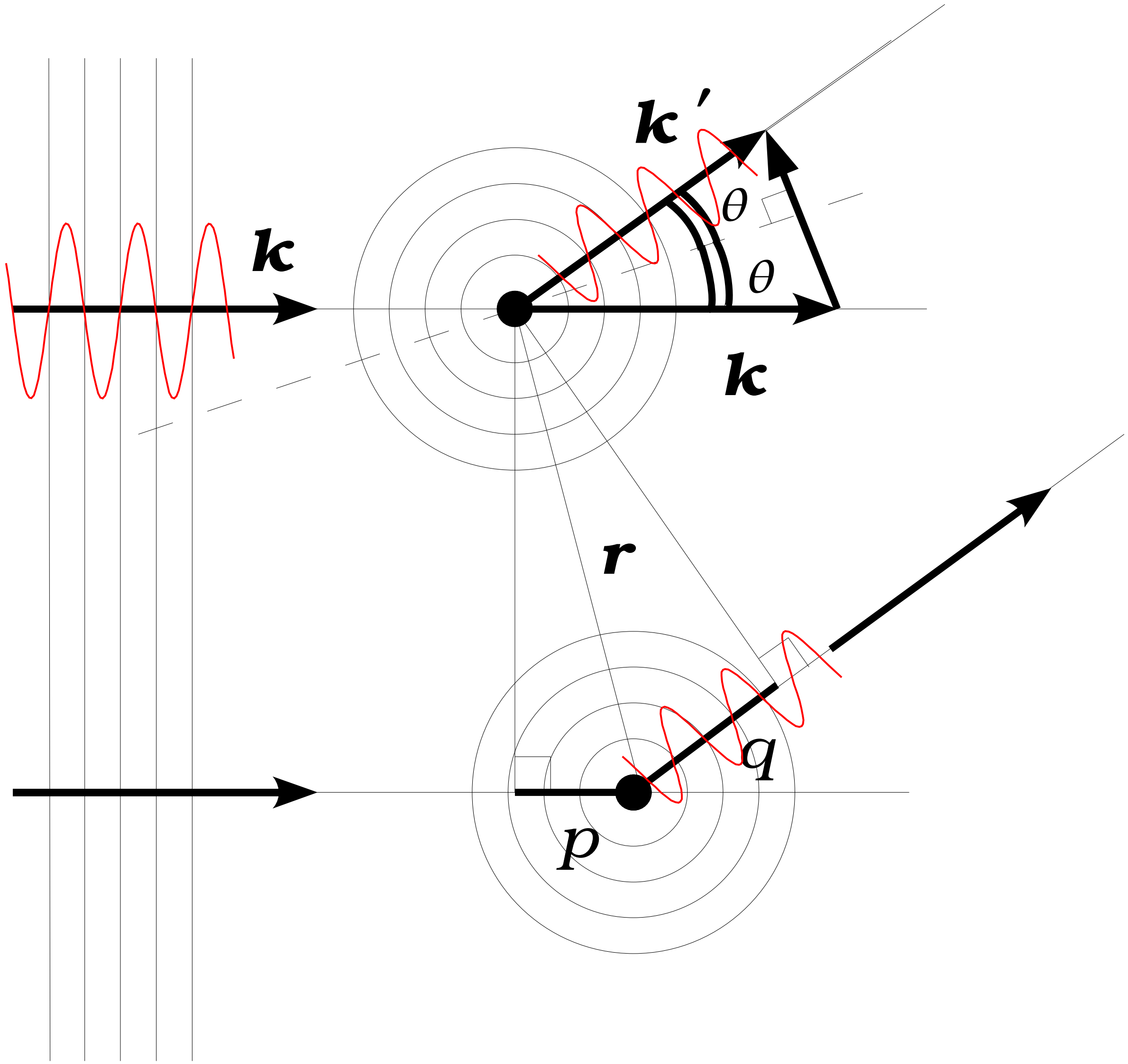
$$|\boldsymbol{k}| = \frac{2\pi}{\lambda}$$

$$\omega = \frac{2\pi}{T}$$

$$E = E_0 \cos(\omega t - \boldsymbol{k}\boldsymbol{x} - \Delta\varphi)$$

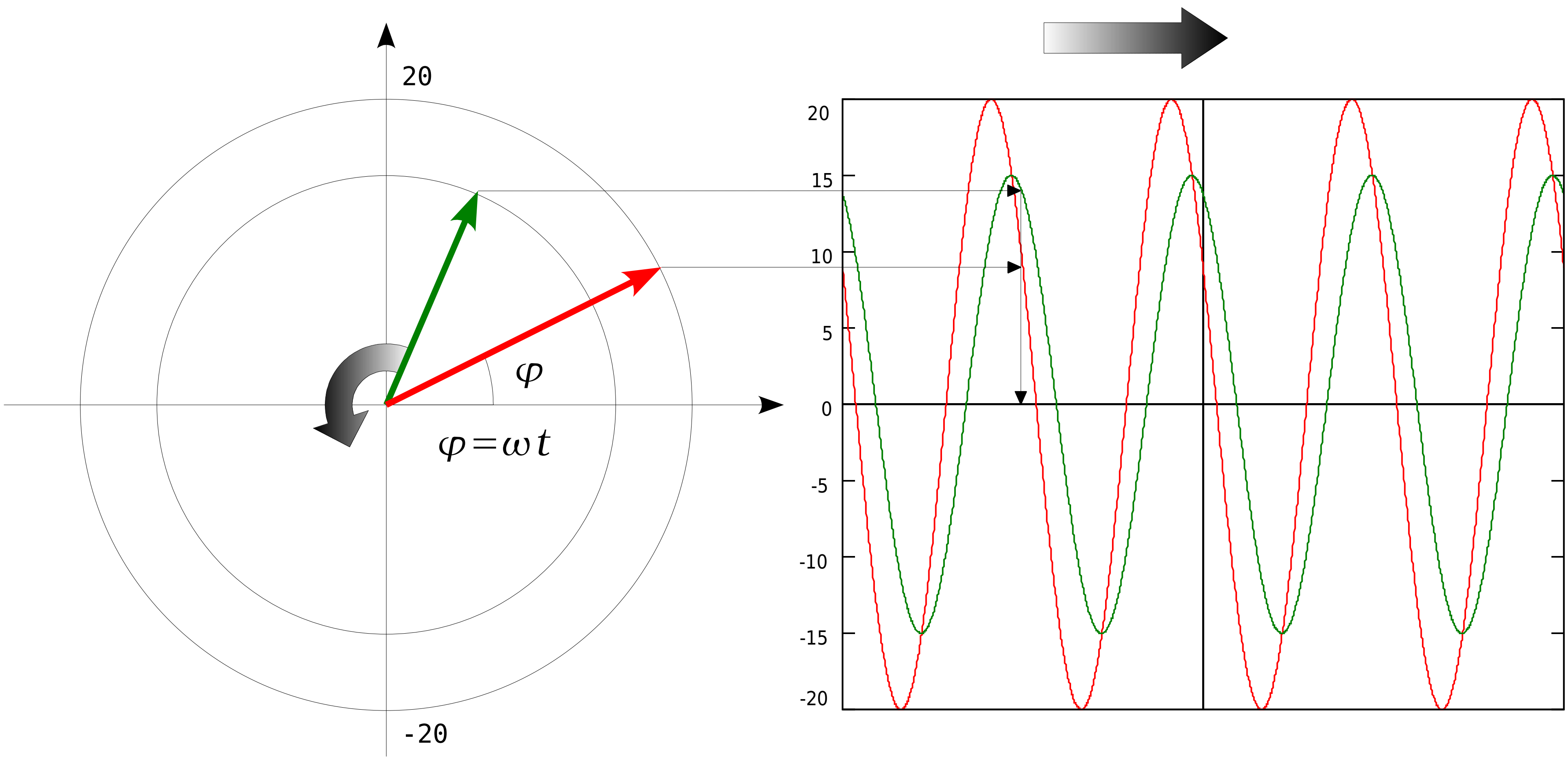
When a flat wave hits charged particles, those start emitting spherical scattered waves.

Scattering of waves (2)



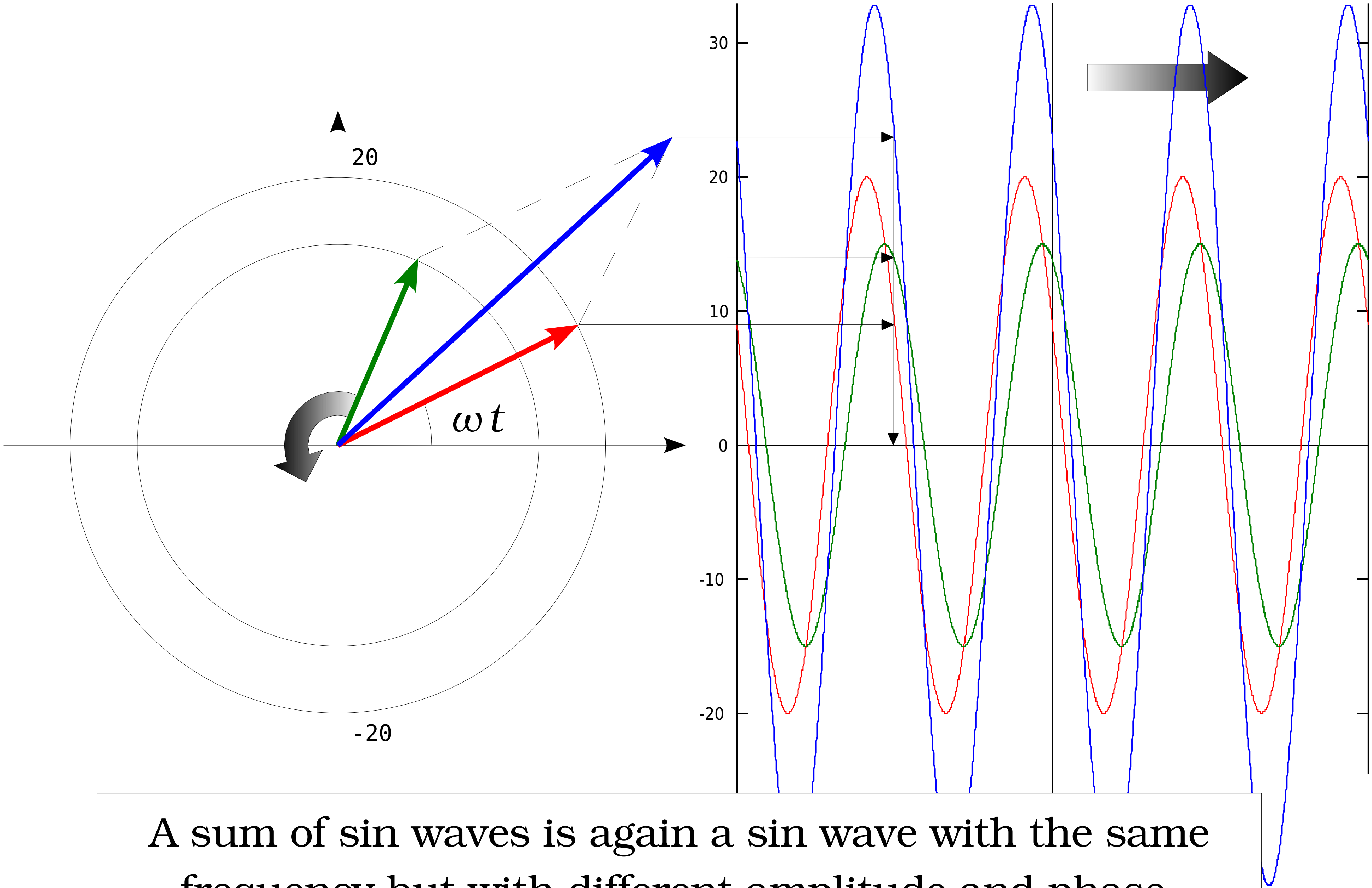
Wave from the particle 2 lags with the phase difference $2\pi\boldsymbol{r}\boldsymbol{S}$.

Addition of sin waves



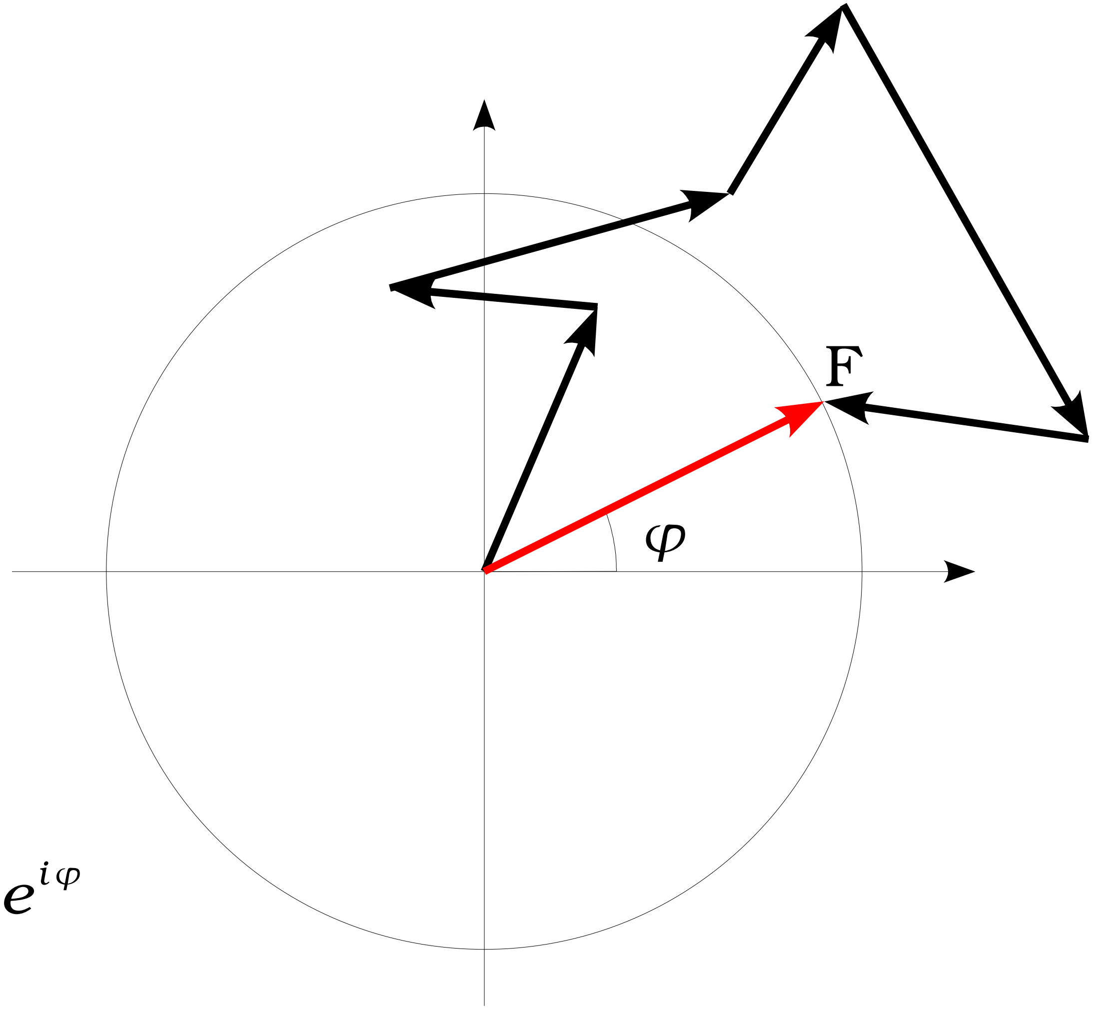
Sin waves can be represented as rotating vectors.

Addition of sin waves (2)



A sum of sin waves is again a sin wave with the same frequency but with different amplitude and phase.

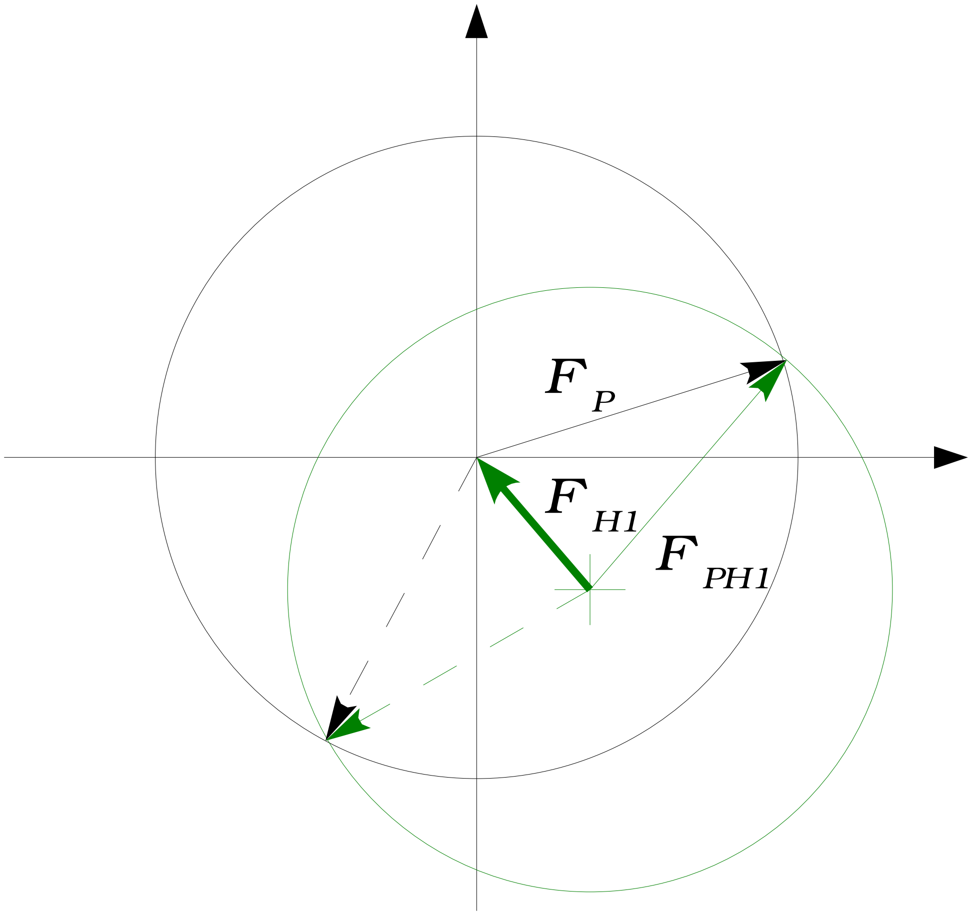
Adding many waves



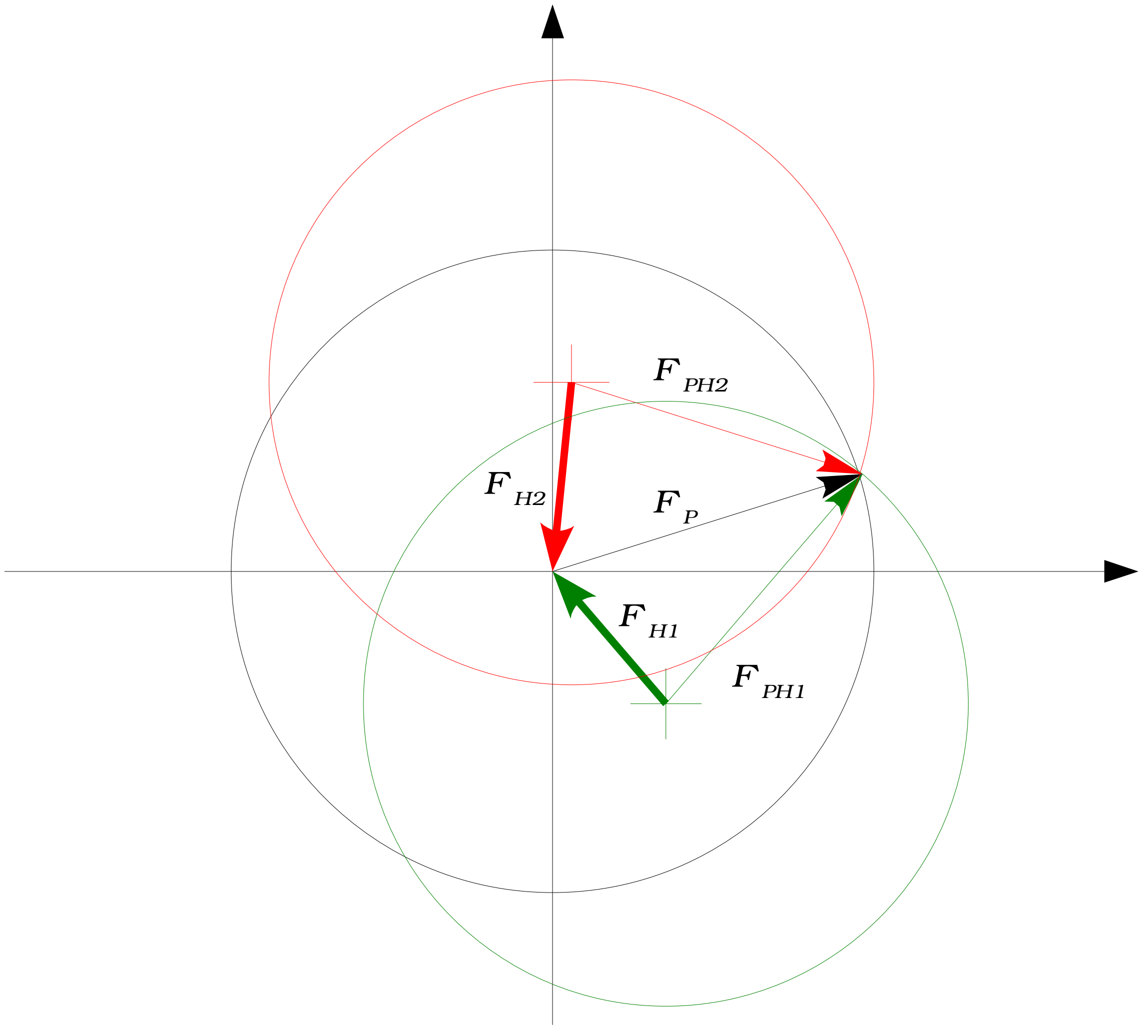
$$F = |F| e^{i\varphi}$$

Multiple sin waves add up, giving a sin wave with some new amplitude and some new phase

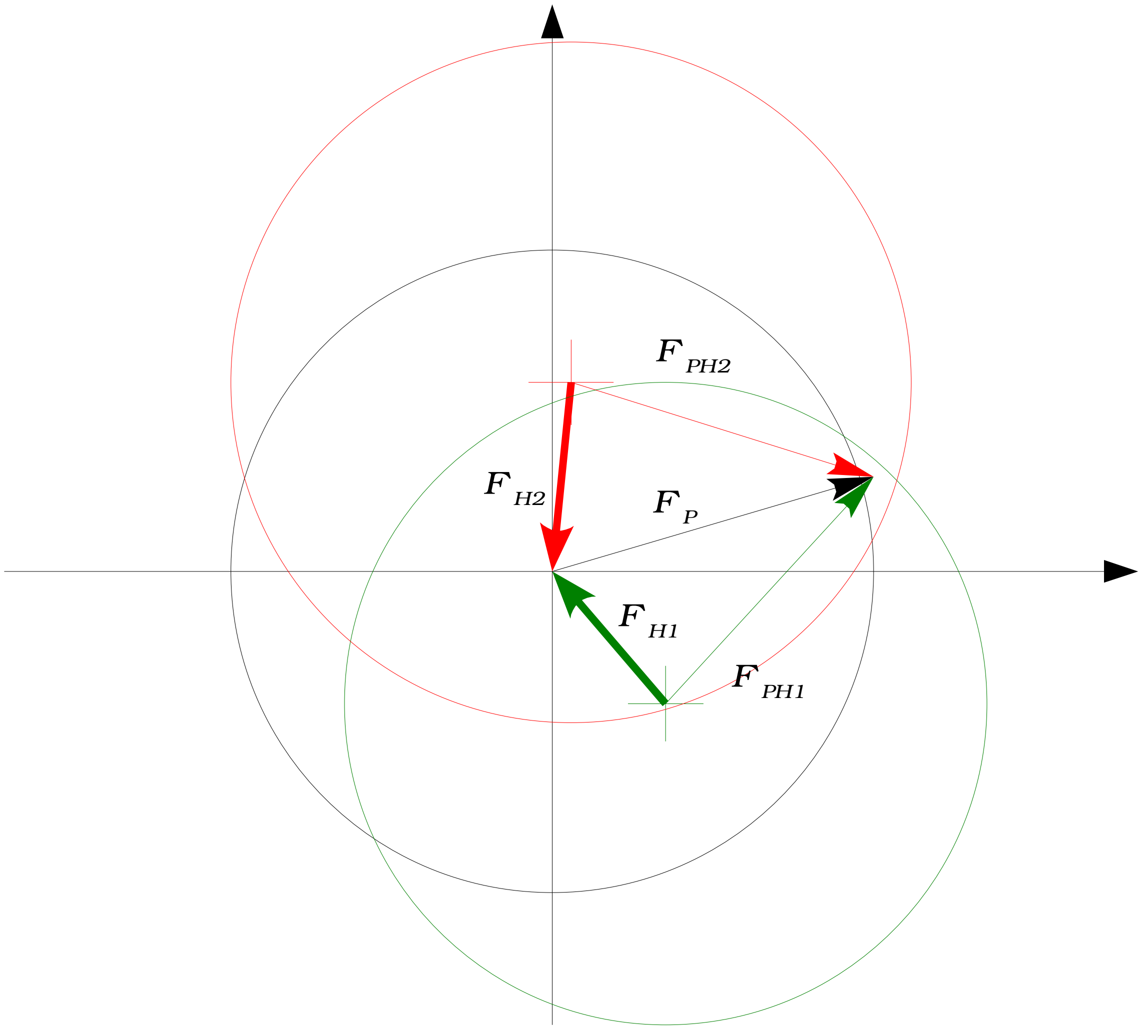
Single Isomorphous Replacement (SIR)



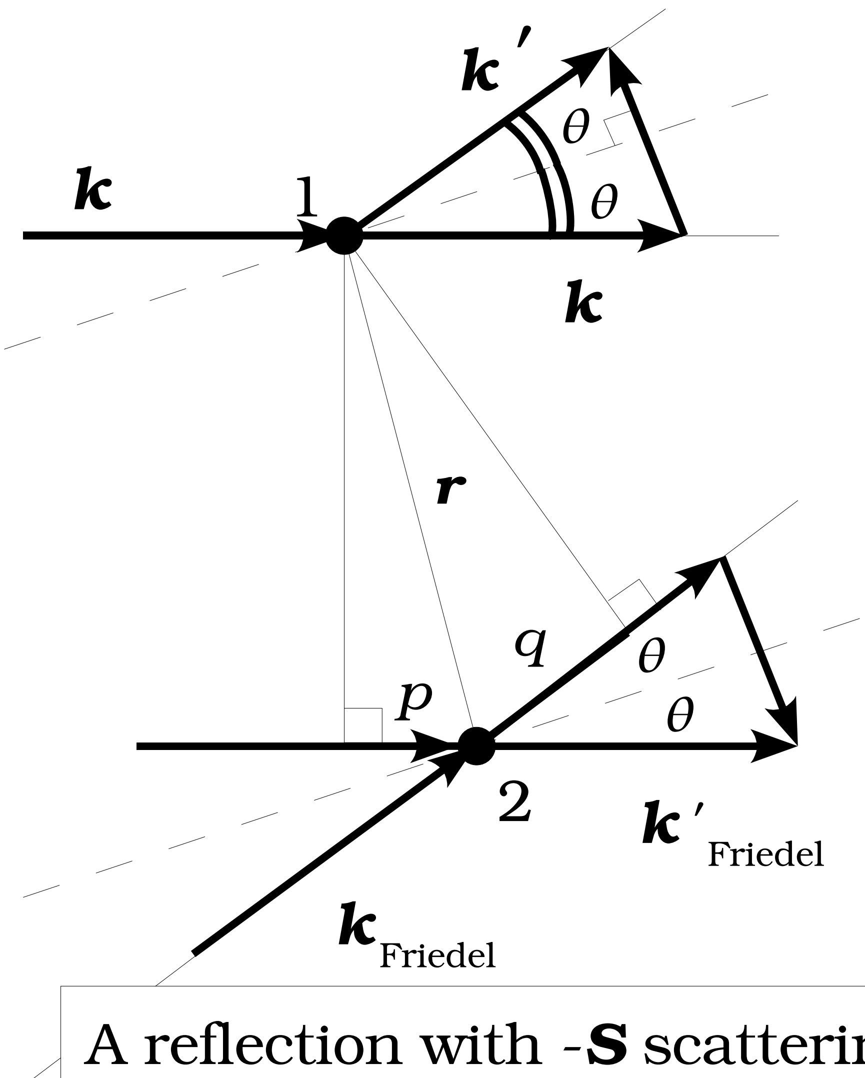
What happens during MIR

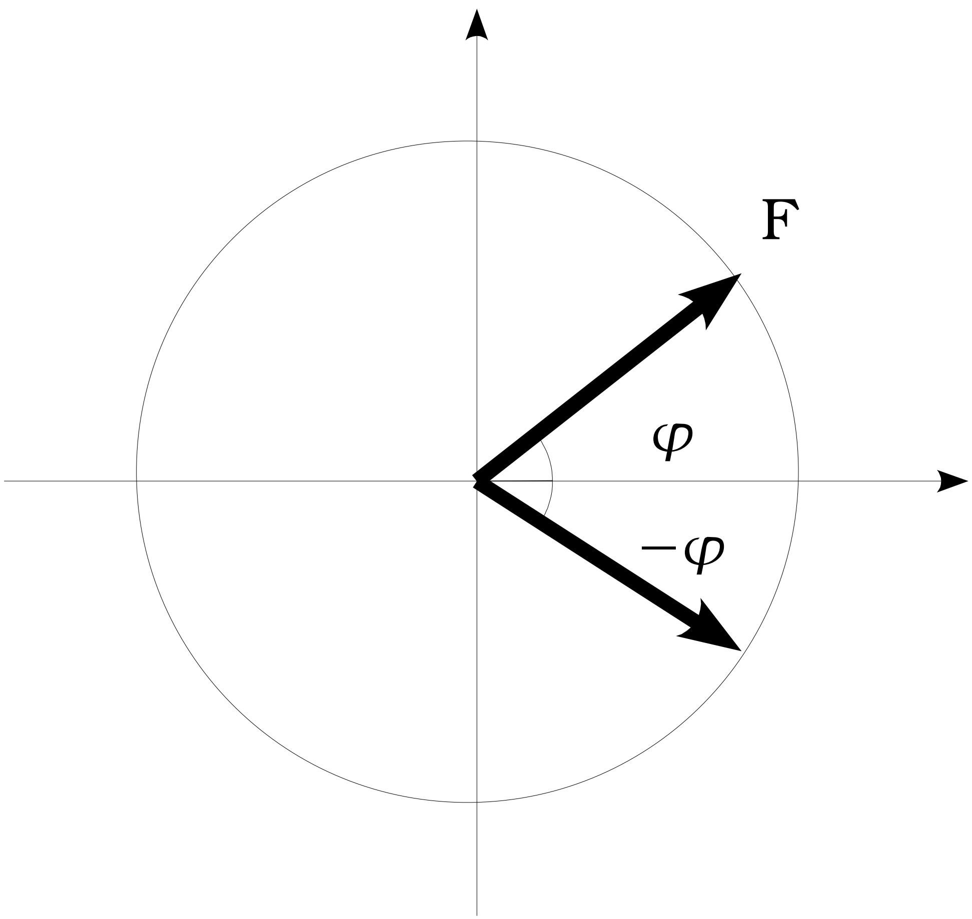


The real life...



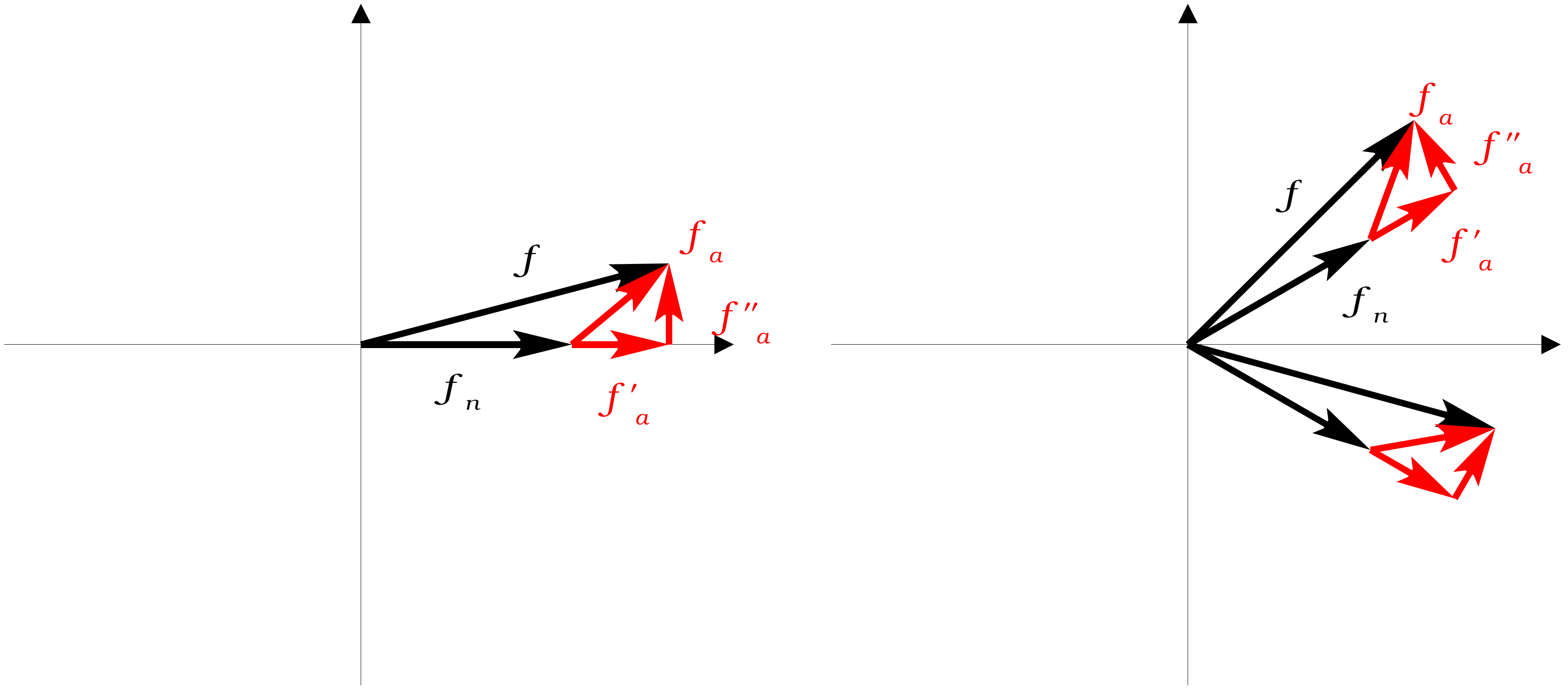
Friedel's law



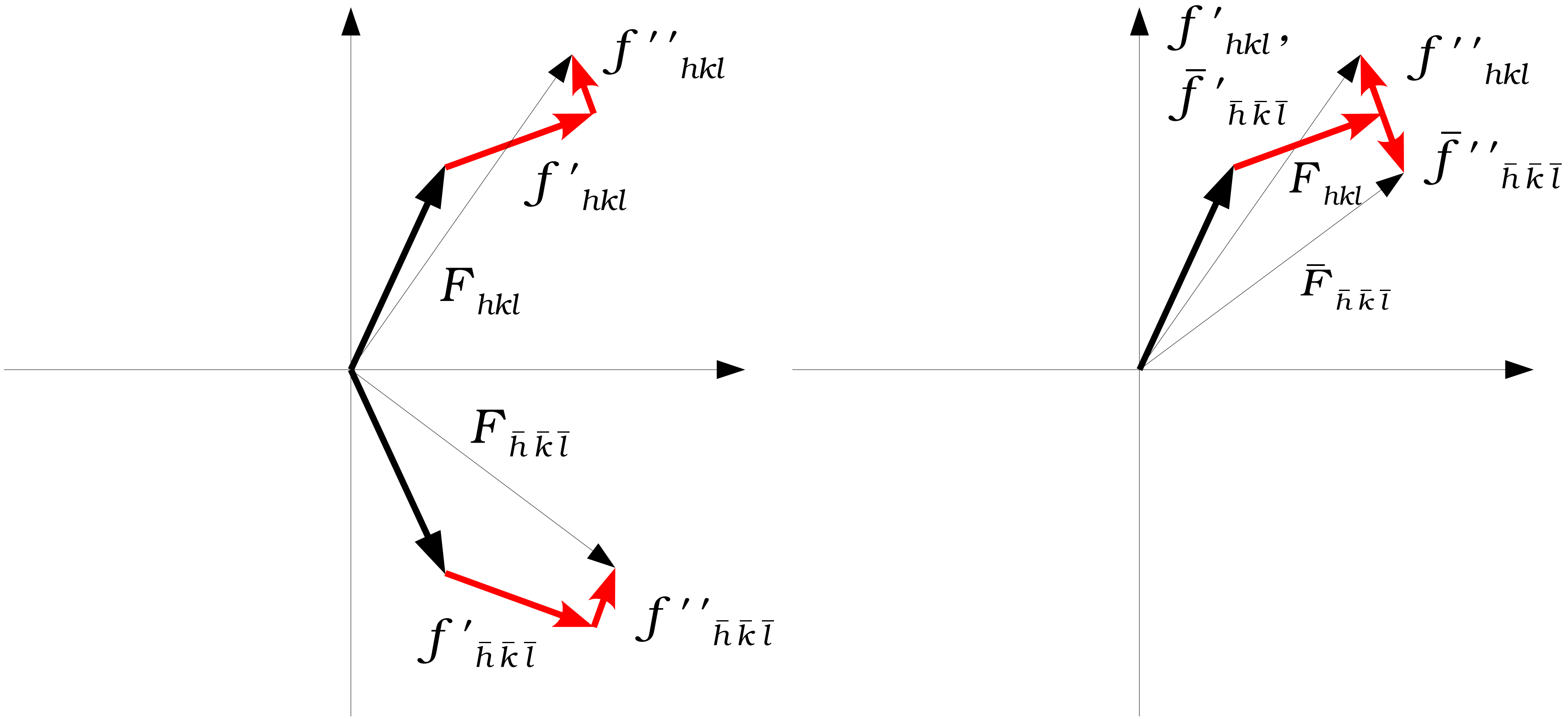


A reflection with -***S*** scattering vector will have the same amplitude but an opposite phase.

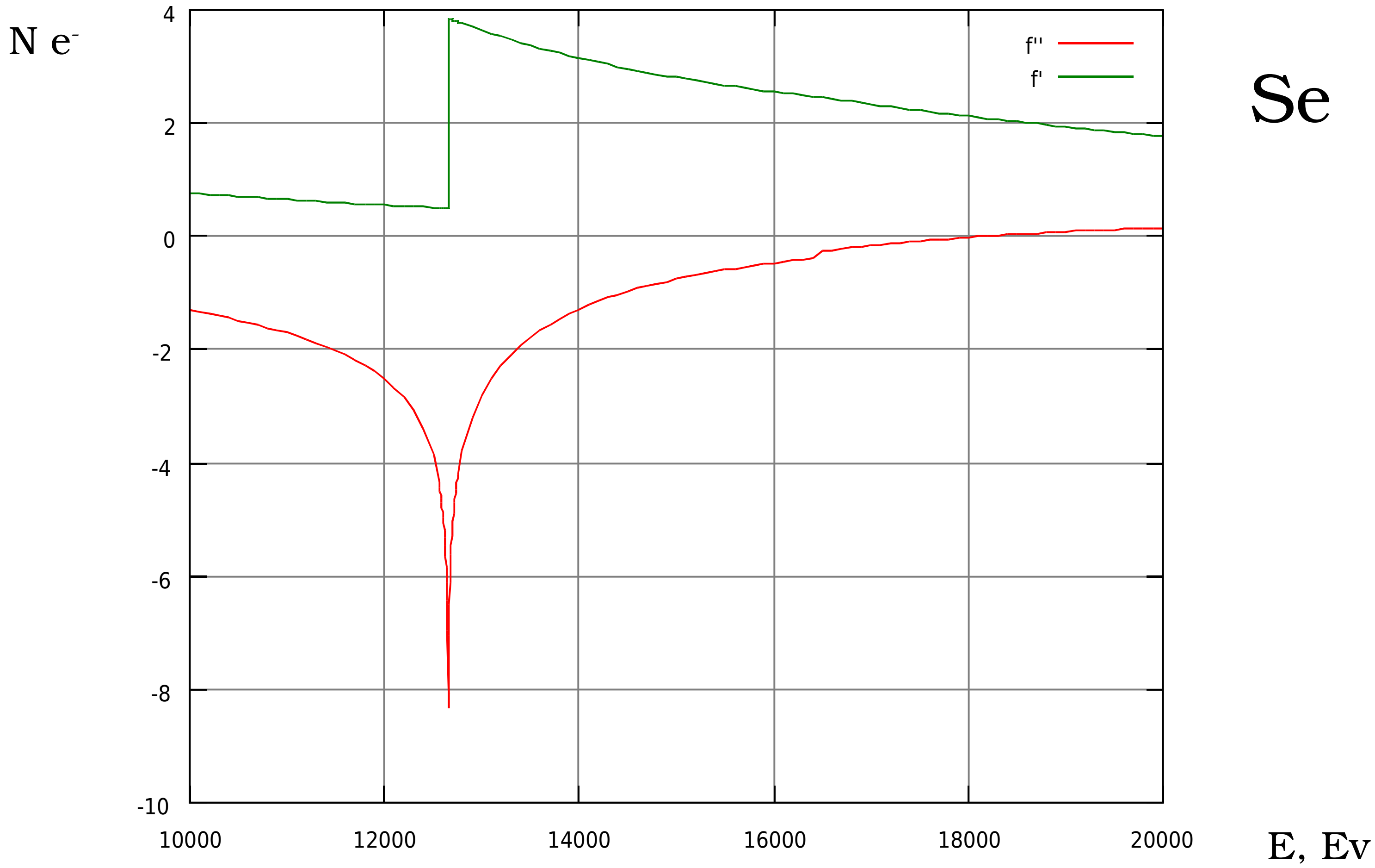
Anomalous scattering



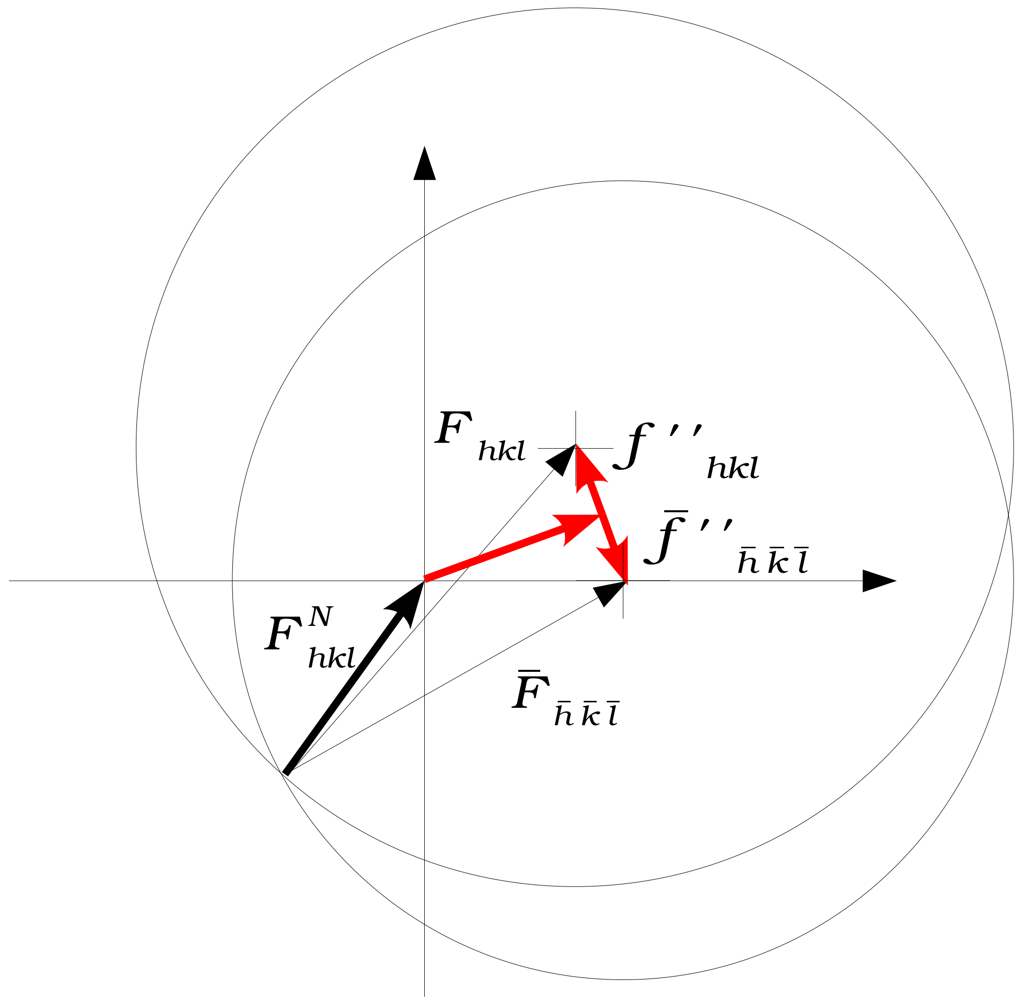
Anomalous difference



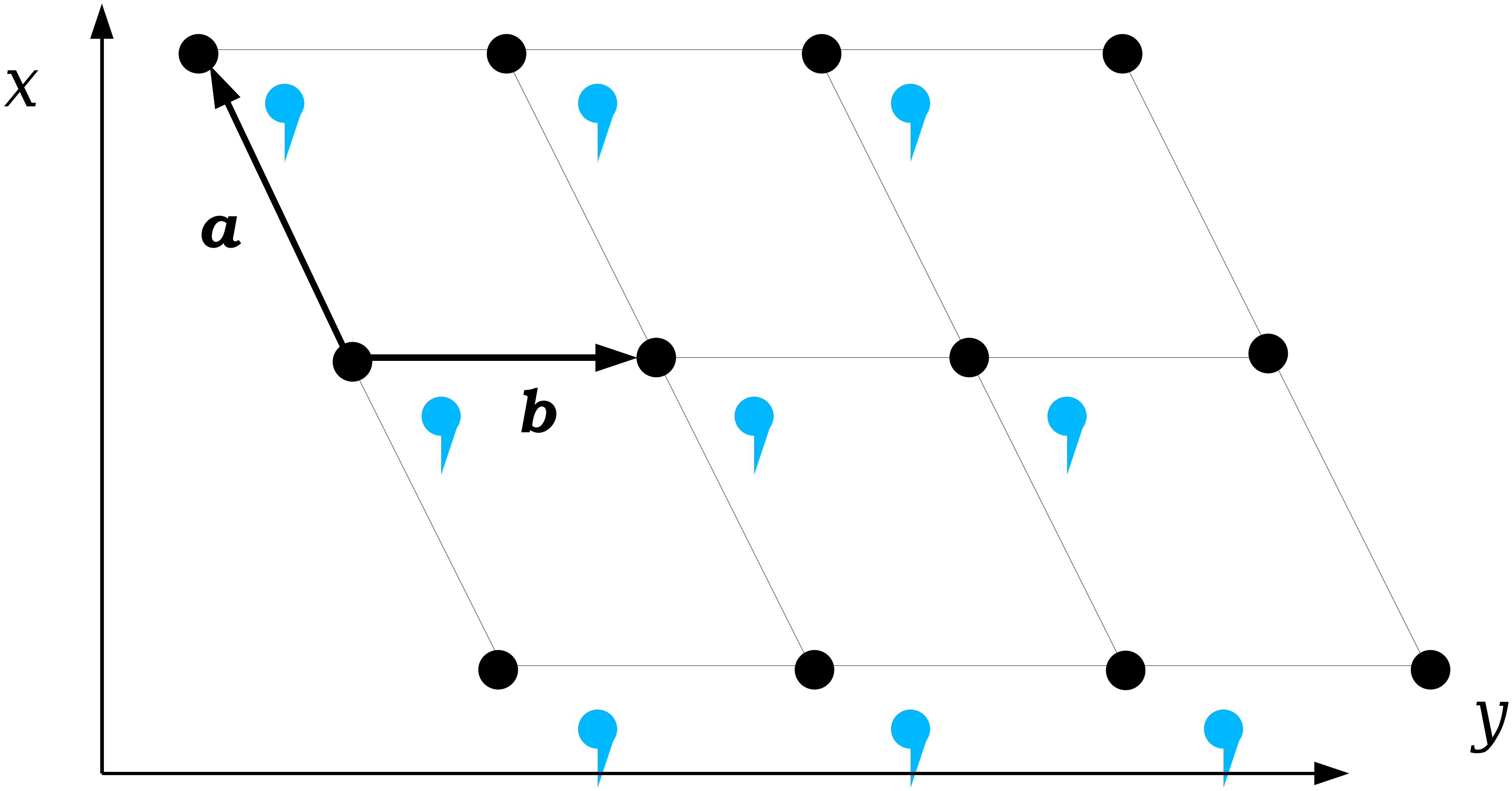
Dependence of the anomalous signal from energy



Anomalous phasing (SAD)

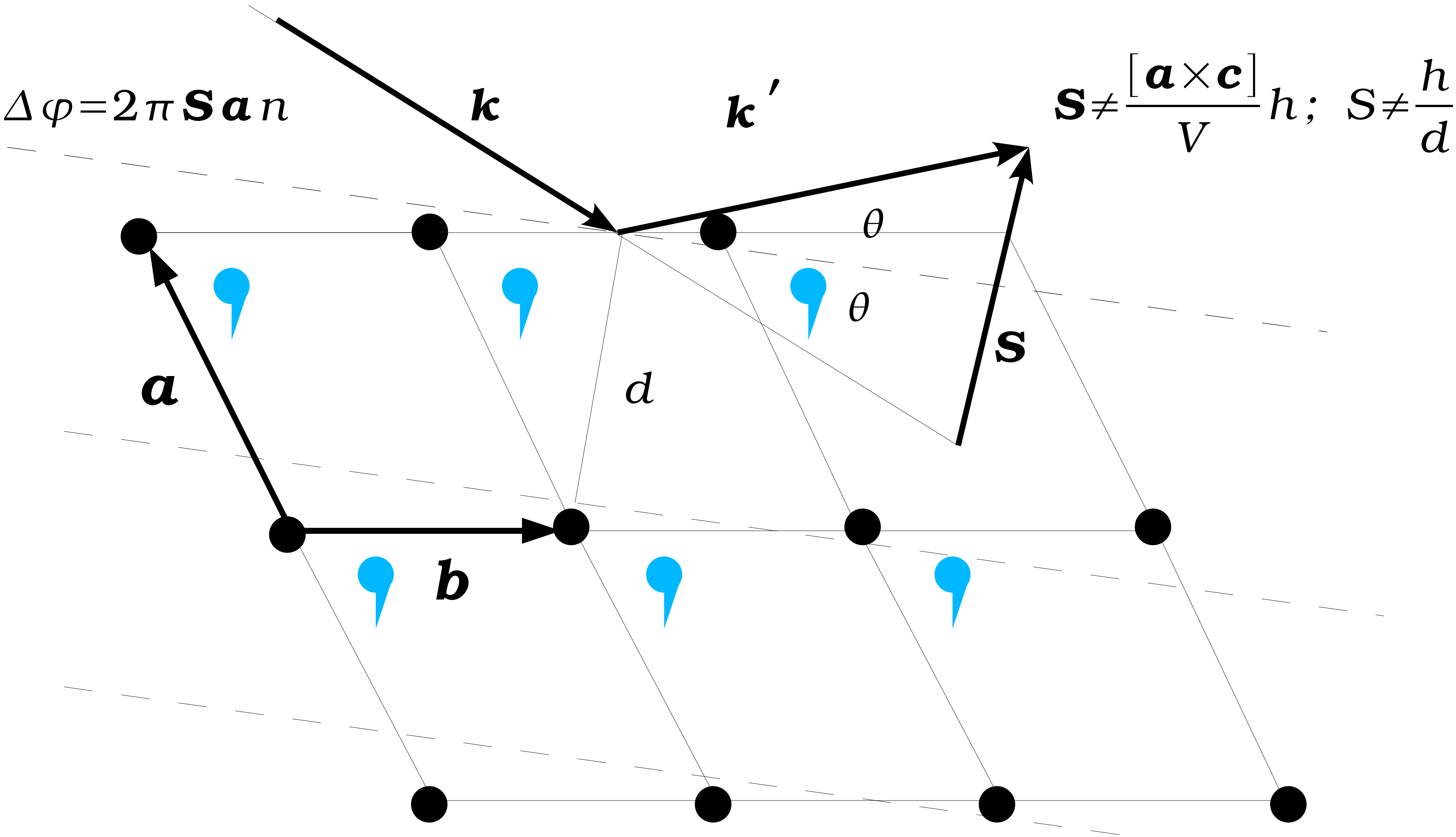


Crystals



A crystal is a periodic array of molecules; its lattice is defined by three **lattice vectors** ***a***, ***b*** and ***c***.

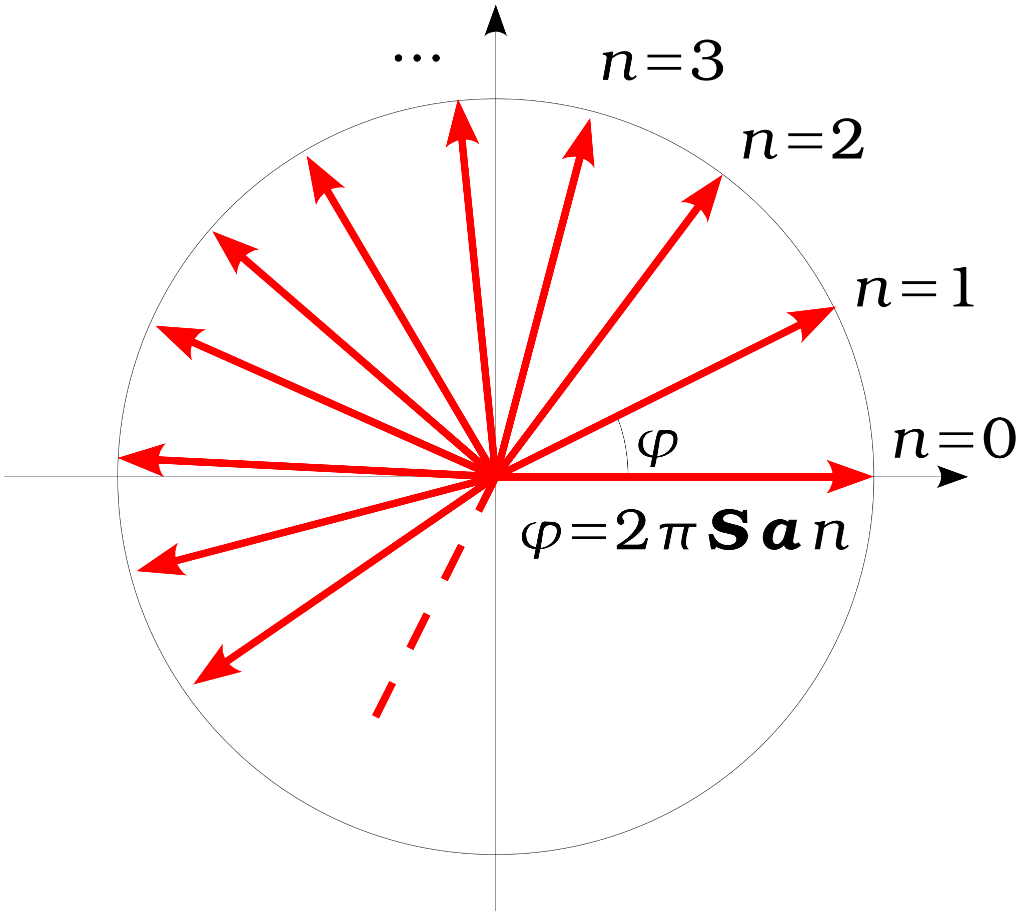
Reflection from a tilted crystal



In a general orientation of a crystal, for every atom in a reflecting plane there is an equivalent atom that scatters out of phase

Reflection from a tilted plain

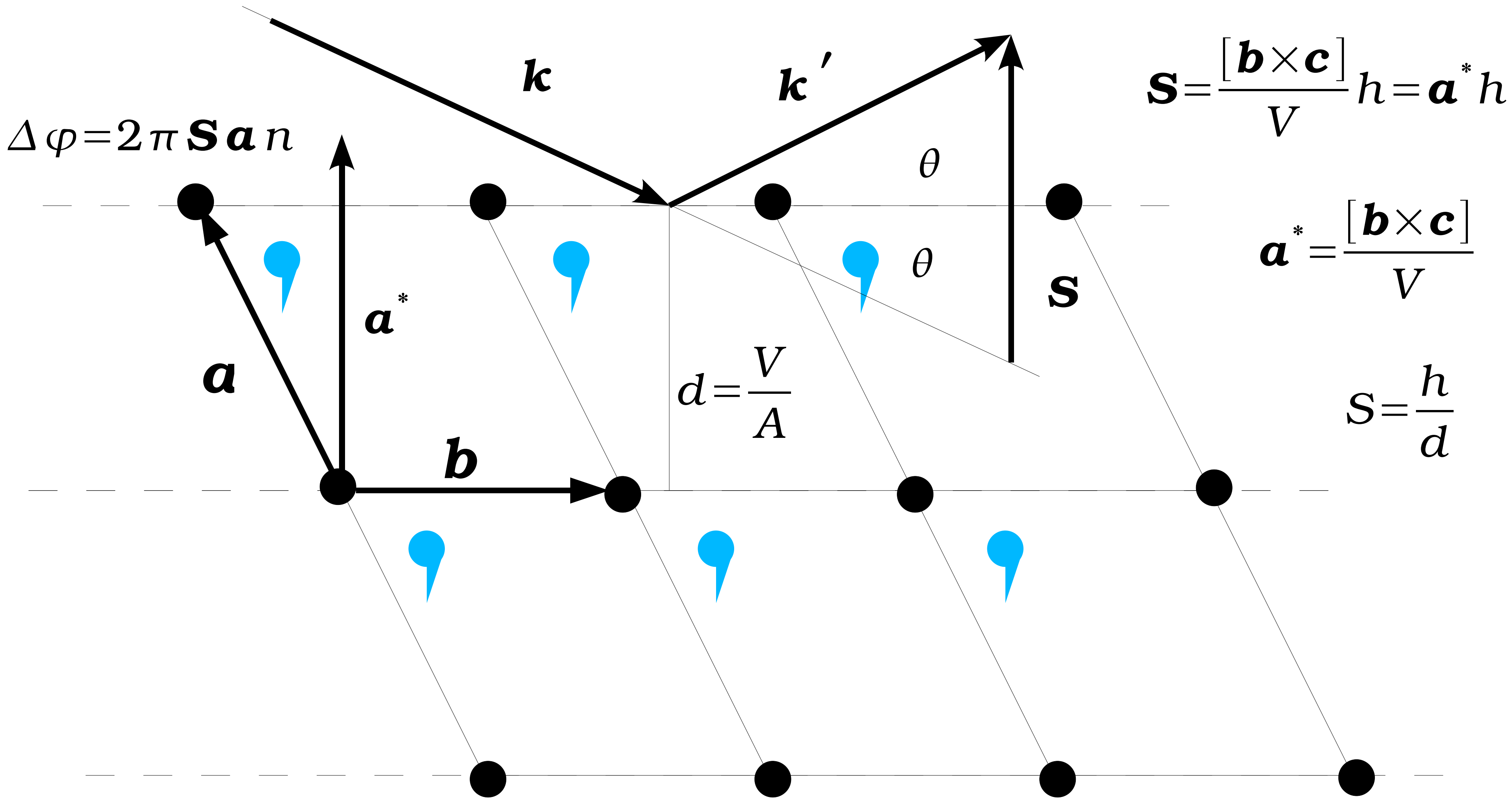
$\boldsymbol{S}\boldsymbol{a} \notin \mathbb{Z}$



Waves from the out-of-planes atoms cancel each other

(Adapted from J. Drenth, "Principles of Protein X-ray Crystallography")

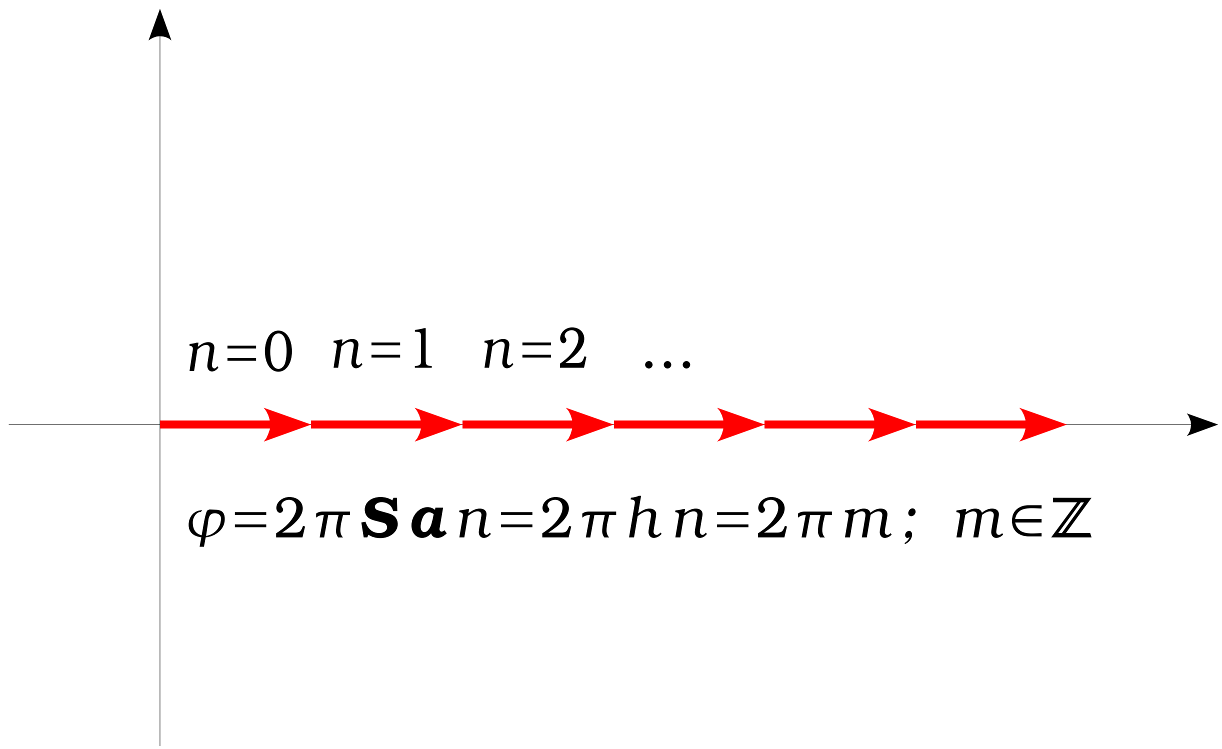
Reflections from a crystal



When a lattice plane coincides with the reflecting plane, all equivalent atoms scatter in phase.

Scattering from a crystal plane

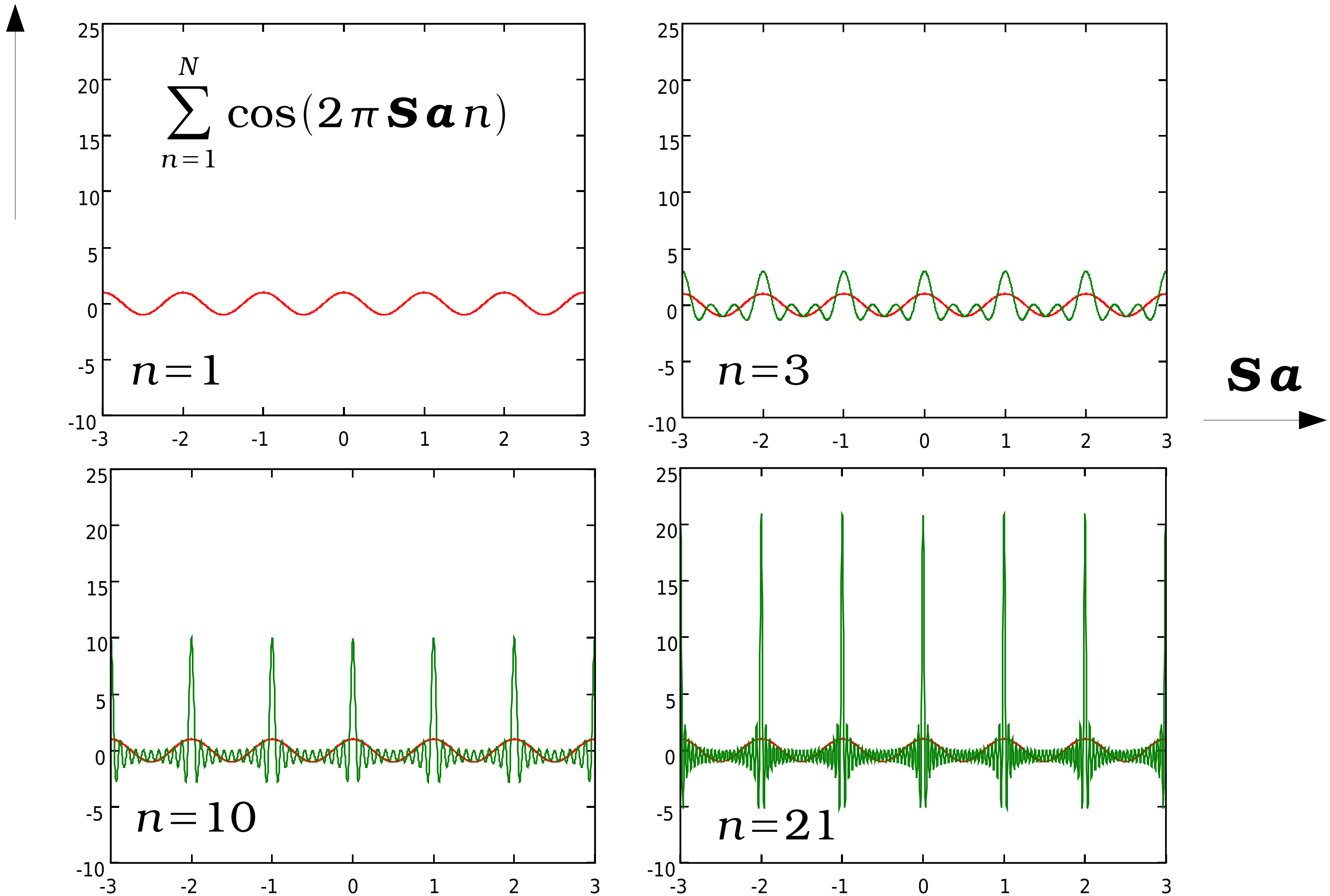
$\boldsymbol{S}\boldsymbol{a}=h;\ h\in\mathbb{Z}$



$$\varphi=2\pi\boldsymbol{S}\boldsymbol{a}n=2\pi hn=2\pi m;\ m\in\mathbb{Z}$$

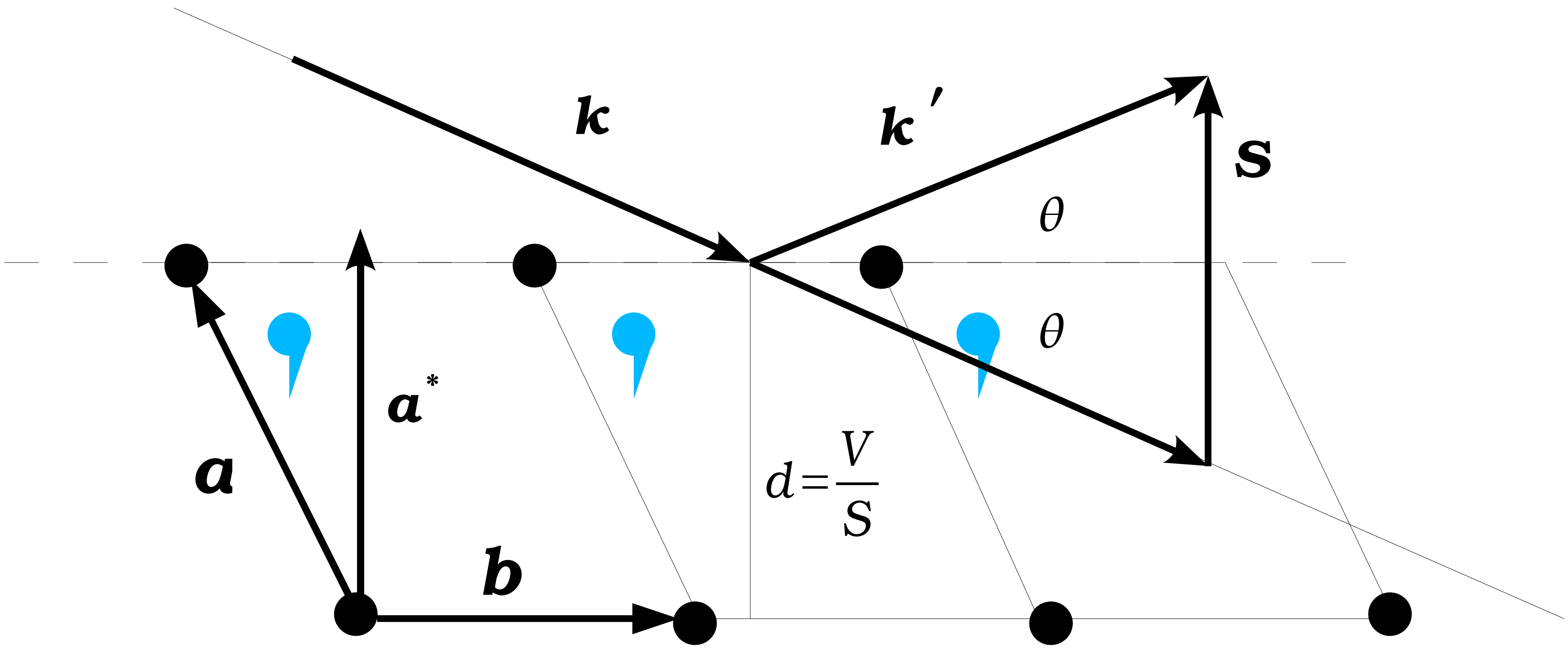
Waves from such the in-phase scattering atoms add up to give an appreciable amplitude.

Example of sin wave addition



Only for integral values of $\boldsymbol{S}\boldsymbol{a}$ the waves add up to give an appreciable intensity.

Scattering from the crystal



1) Laue conditions:

$$\mathbf{S}\,\mathbf{a}=h\,;\ \ \mathbf{S}\,\mathbf{b}=k\,;\ \ \mathbf{S}\,\mathbf{c}=l$$

$$\mathbf{S}=h\,\mathbf{a}^{*}+k\,\mathbf{b}^{*}+l\,\mathbf{c}^{*}$$

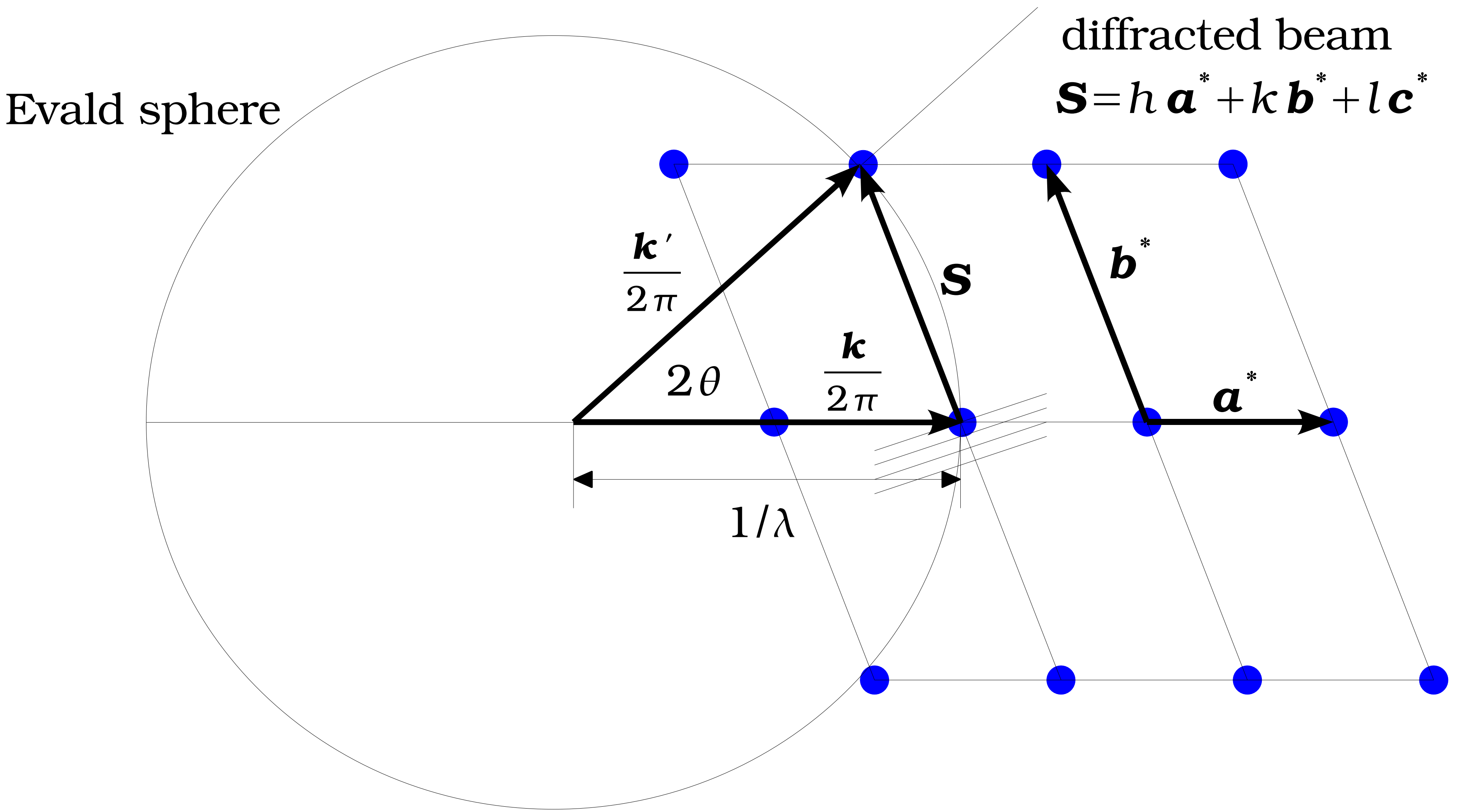
2) Bragg's law:

$$|\mathbf{S}|=\frac{n}{d}=\frac{2\,\sin\theta}{\lambda}$$

$$\mathbf{S}=(\mathbf{k}-\mathbf{k}')/2\pi$$

To get a beam reflected from a crystal, Laue conditions must be satisfied for the chosen Bragg reflection

Ewald's construct



A scattered beam is reflected when a node of the reciprocal lattice lands on the Ewald sphere