Reciprocal lattice for 2D non-square crystal.

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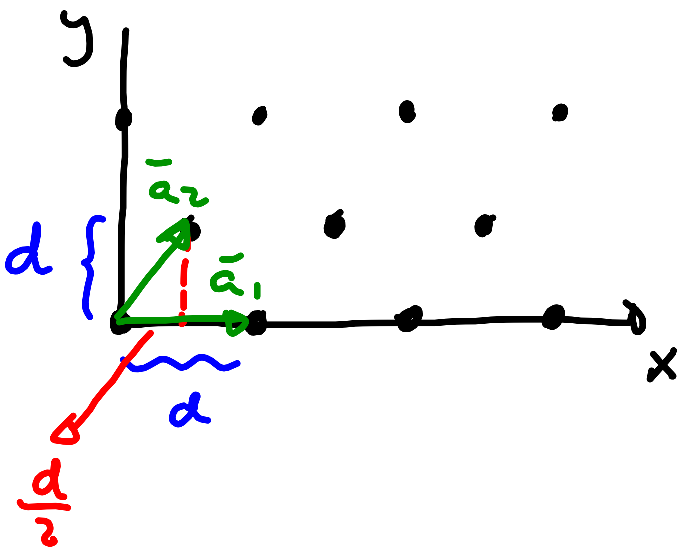
Real space



$\bar{a}_1 = d\,\hat{x}$

$\bar{a}_2 = \frac{d}{2}\hat{x} + d\,\hat{y}$

$|\bar{a}_1| = d$

$|\bar{a}_2| = \frac{\sqrt{5}}{2} d$

$\bar{R} = n_1 \bar{a}_1 + n_2 \bar{a}_2$

We want to find $\bar{b}_1$ and $\bar{b}_2$ so that

$$\bar{K} = m_1 \bar{b}_1 + m_2 \bar{b}_2 .$$

We know that $\bar{K} \cdot \bar{R} = 2\pi n$ (1)

From (1): If $\bar{b}_1 = (b_{1x}, b_{1y})$ $\bar{a}_1 = (d, 0)$

$\bar{b}_2 = (b_{2x}, b_{2y})$ $\bar{a}_2 = (\frac{d}{2}, d)$

$$\left.\begin{aligned} \bar{a}_1 \cdot \bar{b}_1 &= 2\pi \\ \bar{a}_2 \cdot \bar{b}_2 &= 2\pi \\ \bar{a}_1 \cdot \bar{b}_2 &= 0 \\ \bar{a}_2 \cdot \bar{b}_1 &= 0 \end{aligned}\right\} \text{Found last time}$$

$$\bar{a}_1 \cdot \bar{b}_1 = 2\pi = d\, b_{1x} \quad \therefore \quad \boxed{b_{1x} = \frac{2\pi}{d}}$$

$$\bar{a}_2 \cdot \bar{b}_1 = 0 = \frac{d}{2} b_{1x} + d\, b_{1y} = 0$$

$$\frac{\cancel{d}}{\cancel{2}} \frac{2\pi}{\cancel{d}} = -d\, b_{1y} \Rightarrow \boxed{b_{1y} = -\frac{\pi}{d}}$$

$$\boxed{\bar{b}_1 = \frac{2\pi}{d}\left(1, -\frac{1}{2}\right)}$$

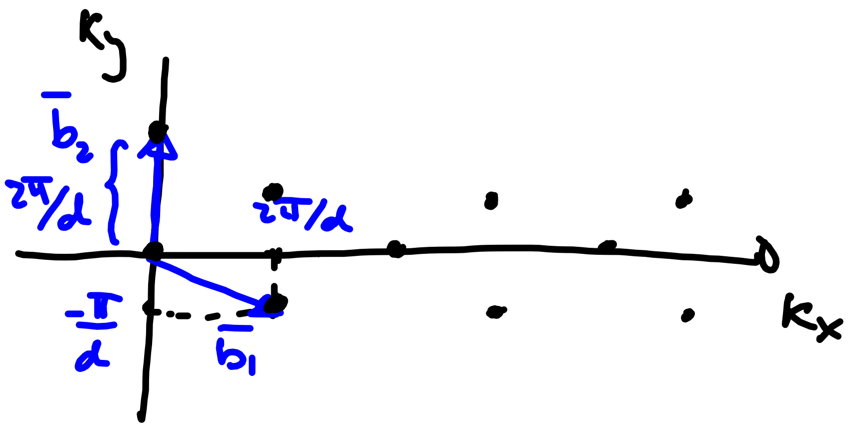
$$\bar{a}_2 \cdot \bar{b}_2 = 2\pi = \frac{d}{2} b_{2x} + d\, b_{2y} \Rightarrow \boxed{b_{2y} = \frac{2\pi}{d}}$$

$$\bar{a}_1 \cdot \bar{b}_2 = 0 = d\, b_{2x} = 0 \Rightarrow \boxed{b_{2x} = 0}$$

$$\boxed{\bar{b}_2 = \frac{2\pi}{d}(0, 1)}$$

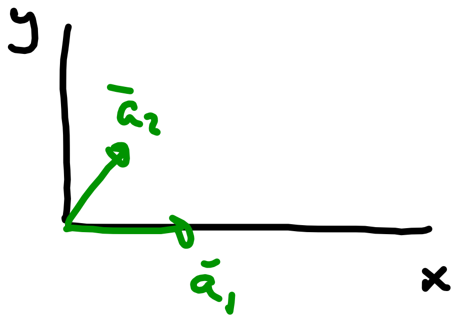
We see that in reciprocal space we have.

$$\bar{b}_1 = \frac{2\pi}{d}\left(1, -\frac{1}{2}\right) \qquad \bar{b}_2 = \frac{2\pi}{d}(0, 1)$$



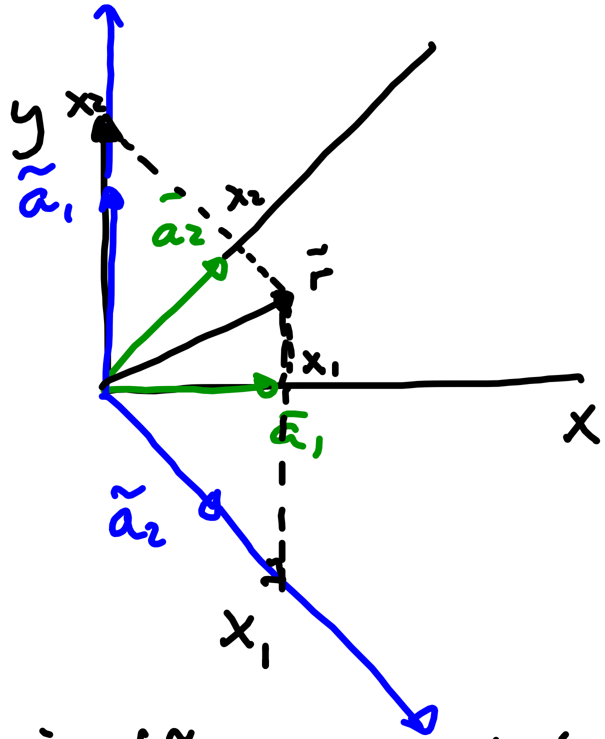
$\bar{b}_2 \perp \bar{a}_1$

$\bar{b}_1 \perp \bar{a}_2$



Dual space for $\bar{a}_i$

(we'll do a numerical example later).



Notice that in real base

x_1 is in units of $\bar{a}_1$.

In dual space x_1 is in units of $\tilde{a}_2$.

When the units are considered you'll see that x_1 is the same in both systems

To find $\{\tilde{a}_i\}$ use that

$$\boxed{\tilde{a}^i a_j = \delta^i_j}$$

not 2π factor.

If you write $\bar{r} = x_i \tilde{a}^i = x_1 \tilde{a}^1 + x_2 \tilde{a}^2$

you will find that $x_i \equiv x'_{i\perp}$

Covariant and Contravariant Vectors.

We have defined our prototype contravariant vector $r^i = \bar{r}$ that transforms like

$$r'^i = \frac{\partial x'^i}{\partial x^j} r^j$$

going from a system K to a system K'.

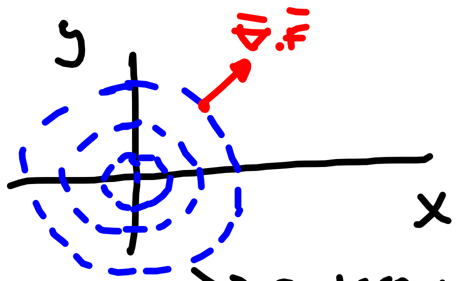
Now we will see how the gradient of a scalar function transforms going from K to K'.

Gradient

The gradient of a scalar field $F(x,y)$ is a vector.

$$\bar{\nabla} F(x,y) = \frac{\partial F}{\partial x}\hat{x} + \frac{\partial F}{\partial y}\hat{y} = \left(\frac{\partial F}{\partial x}, \frac{\partial F}{\partial y}\right) \equiv$$

$$\equiv \left(\frac{\partial F}{\partial x^1}, \frac{\partial F}{\partial x^2}\right)$$



surface where $F(\bar{r})$ is constant

The gradient at point P is a vector perpendicular to a surface where F is constant.

In tensor notation:

$$\bar{\nabla} F = \frac{\partial F}{\partial x^i} = B_i \equiv \bar{B}$$

I wrote the index down because x^i is downstairs. So this "hints" that $\bar{B}$ will be covariant.

We know that going from K to K'

$$r'^i = \frac{\partial x'^i}{\partial x^j} r^j$$

For $\bar{B}$ we obtain:

$$\underbrace{\bar{\nabla}' F'(x', y')}_{\text{in } K'} = \bar{B}' = (B'_{x'}, B'_{y'}) = \left(\frac{\partial F(x', y')}{\partial x'}, \frac{\partial F(x', y')}{\partial y'} \right)$$

since $F(x,y)$ is a scalar it means that

$F(x'^1,y') = F(x,y)$ whe x'^i are the coordinates of r^i in K' and x^i in K. Then

$$\bar{\nabla}' F(x',y') = \bar{B}' = \left(\frac{\partial F(x,y)}{\partial x'}, \frac{\partial F(x,y)}{\partial y'} \right) =$$

$$= \left(\overbrace{\frac{\partial F(x,y)}{\partial x}}^{B_x} \frac{\partial x}{\partial x'} + \overbrace{\frac{\partial F(x,y)}{\partial y}}^{B_y} \frac{\partial y}{\partial x'}, \right.$$

$$\left. \overbrace{\frac{\partial F(x,y)}{\partial x}}^{B_x} \frac{\partial x}{\partial y'} + \overbrace{\frac{\partial F(x,y)}{\partial y}}^{B_y} \frac{\partial y}{\partial y'} \right) =$$

$$= \left(B_x \frac{\partial x}{\partial x'} + B_y \frac{\partial y}{\partial x'},\ B_x \frac{\partial x}{\partial y'} + B_y \frac{\partial y}{\partial y'} \right)$$

In tensor form it becomes:

$$B'_i = B_j \frac{\partial x^j}{\partial x'^i}$$

or

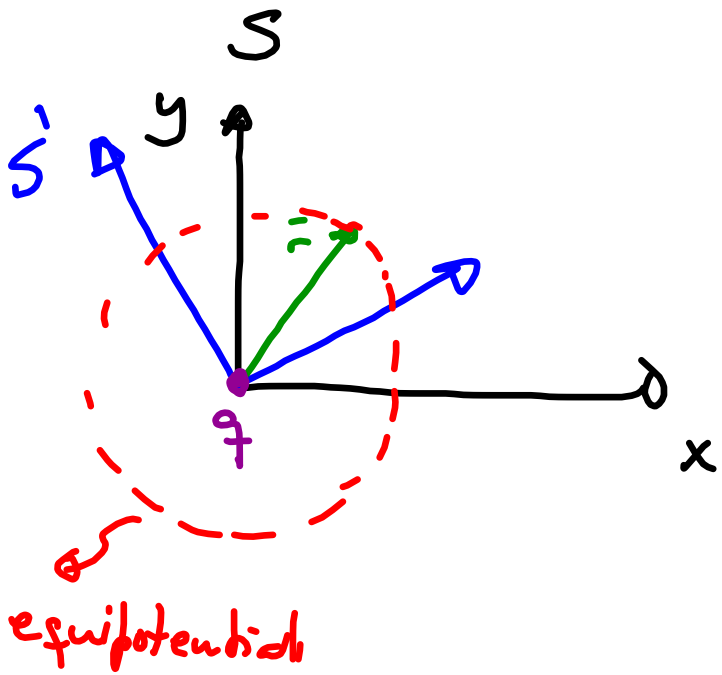
$$\boxed{B'_i = \frac{\partial x^j}{\partial x'^i} B_j}$$

covariant transformation

The gradient of a scalar field is the prototype covariant vector.

Example of covariant vector:

Electric field (in 2D)



In S:

$$V(x,y) = V(r) = \frac{1}{4\pi\varepsilon_0 r} \equiv \frac{A}{r}$$

In S':

$$V'(x',y') = V(r') = \frac{1}{4\pi\varepsilon_0 r'} \equiv \frac{A}{r}$$

$r = r'$ scalar.

To obtain $\bar{E}$ at $\bar{r}$ you calculate

$$\bar{E} = -\bar{\nabla} V.$$

In S:

$$\bar{E}(x,y) = -\bar{\nabla} V(x,y) =$$

$$= (E_x, E_y) = \left(-\frac{\partial V}{\partial x}, -\frac{\partial V}{\partial y}\right) = \frac{A}{r^3}(x,y)$$

In S':

$$\bar{E}'(x',y') = \left(-\frac{\partial V}{\partial x'}, -\frac{\partial V}{\partial y'}\right) = \frac{A(x',y')}{r^3}$$

The components are functions of different coordinates

$$E'_i = -\frac{\partial V'}{\partial x'^i} = \underbrace{-\frac{\partial V}{\partial x^j}}_{E_j} \frac{\partial x^j}{\partial x'^i} = E_j \frac{\partial x^j}{\partial x'^i}$$

covariant vector.

$[V] = \text{volts}$

$[\bar{E}] = \frac{\text{volts}}{\text{meter}}$

$\bar{E}$ has units of length^{-1} which is typical of physical covariant vectors.

Now let's verify that $-\nabla V$ provides the covariant components of $\bar{E}$ using an oblique system for K':

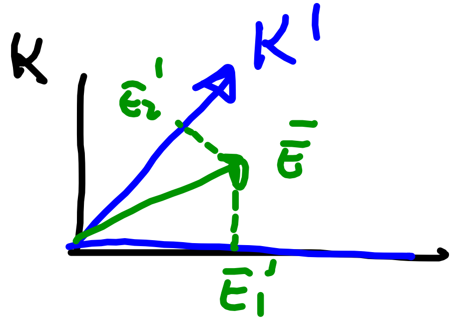
In K': $\quad E'_i = E_j \dfrac{\partial x^j}{\partial x'^i} \qquad \underbrace{A^j{}_i = \dfrac{\partial x^j}{\partial x'^i}}$

$$\therefore \quad (E'_1, E'_2) = (E_1, E_2)\begin{pmatrix} 1 & \cos\alpha \\ 0 & \sin\alpha \end{pmatrix} \Rightarrow$$

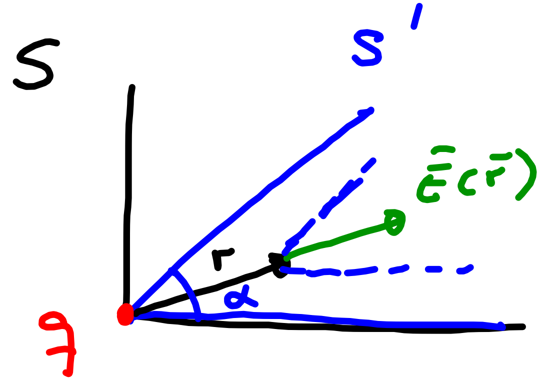
$E'_1 = E_1$

$E'_2 = E_1 \cos\alpha + E_2 \sin\alpha$

$E'_i = -\nabla' V' = -\partial'_i V$



Formal derivation:



We found that

$$\begin{cases} x_1' = x_1 \\ x_2' = \cos\alpha\, x_1 + \sin\alpha\, x_2 \end{cases} \quad (1)$$

and

$$\begin{cases} x_1 = x^{1\prime} + x^{2\prime}\cos\alpha \\ x_2 = x^{2\prime}\sin\alpha \end{cases} \quad (2)$$

From (1) and (2) we can find x'_i in terms of x'^i:

$$\begin{cases} \boxed{x_1' = x^{1\prime} + x^{2\prime}\cos\alpha} \\ \boxed{x_2'} = \cos\alpha\, x^{1\prime} + \cos^2\alpha\, x^{2\prime} + \sin^2\alpha\, x^{2\prime} = \boxed{x^{1\prime}\cos\alpha + x^{2\prime}} \end{cases} \quad (3)$$

From (3) I see that

$$x'_i = g_{ij}\, x'^j \qquad \text{with} \qquad g_{ij} = \begin{pmatrix} 1 & \cos\alpha \\ \cos\alpha & 1 \end{pmatrix}$$

In S:

$$V(\bar{r}) = \frac{q}{4\pi\varepsilon_0 r} = \frac{q}{4\pi\varepsilon_0 (x_i x^i)^{1/2}}$$

In S':

$$V(\bar{r}') = \frac{q}{4\pi\varepsilon_0 r'} = \frac{q}{4\pi\varepsilon_0 (x'_i x'^i)^{1/2}}$$

$$V(\bar{r}) = V(\bar{r}')$$

Then in S':

$$E'_j = -\partial'_j V' = -\frac{\partial V'}{\partial x'^j} = -\frac{q}{4\pi\varepsilon_0}\frac{\partial}{\partial x'^j}\left[\frac{1}{(x'_i x'^i)^{1/2}}\right]$$