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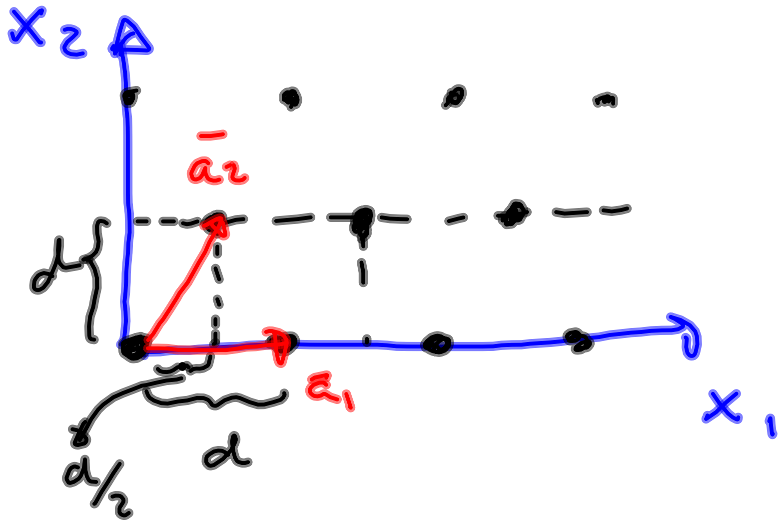
Covariant and contravariant basis:

For each system defined in real space by a covariant bases there is a contravariant basis that is orthogonal to the covariant basis. The contravariant basis is defined in the dual or reciprocal space.

Dual space and dual basis in a 2D crystal: Oblique Bravais lattice.



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

$\bar{a}_2 = \frac{d}{2}\hat{e}_1 + d\,\hat{e}_2$

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

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

$\bar{R} = m_1\bar{a}_1 + m_2\bar{a}_2$ all the points in the lattice.

Let's find $\bar{b}_i \equiv \bar{b}^i$ the basis of the reciprocal lattice.

We know that in the reciprocal lattice a vector $\bar{K}$ is given by:

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

we want $\bar{K} \cdot \bar{R} = 2\pi n$ ①

we found that ① means that

$$a_i b^j = 2\pi \delta_i^j$$

(2π replaced by 1 for a "mathematical" system as in HW)

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If $\bar{b}_1 = (b_{1x}, b_{1y})$ and $\bar{b}_2 = (b_{2x}, b_{2y})$

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

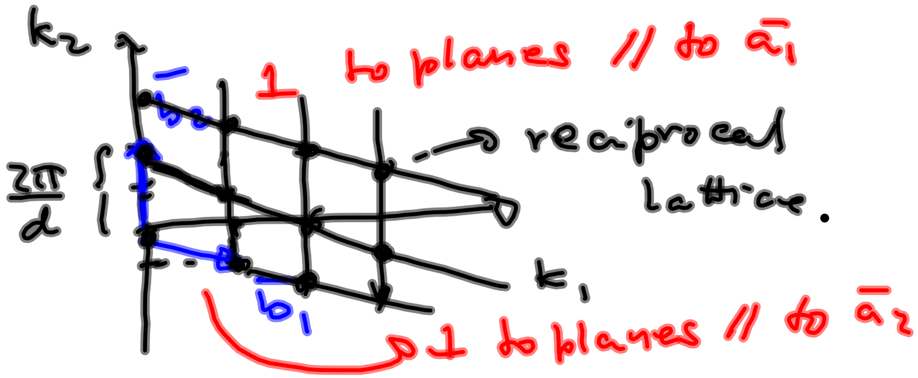
$$\bar{a}_2 \cdot \bar{b}_2 = \frac{d}{2} \cancel{b_{2x}} + d\, b_{2y} = 2\pi \Rightarrow \boxed{b_{2y} = \frac{2\pi}{d}}$$

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

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

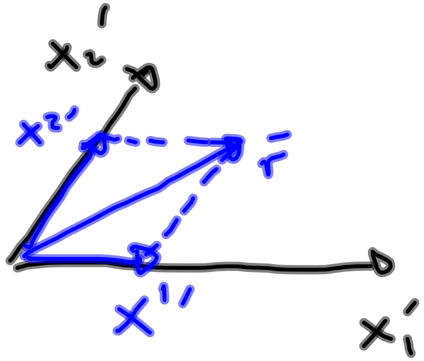
$$\bar{b}_1 = \frac{2\pi}{d}\left(1, -\frac{1}{2}\right)$$

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



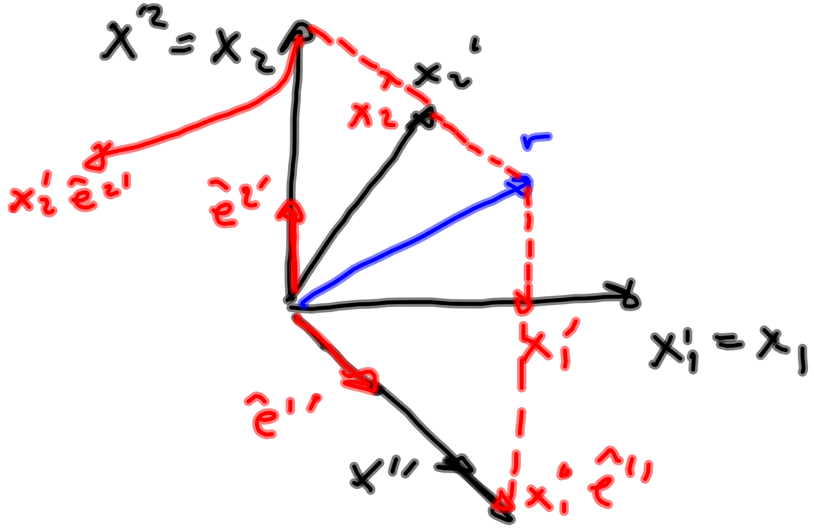
In homework you will show that:

$\bar{r}' = x'^i \hat{e}'_i$ in real space.



and

$\bar{r}' = x'_i \hat{e}'^i$ in dual space.



$\hat{e}^{i'}$ are NOT unit vectors

In dual space and rescaled by $\hat{e}'^i$ the ⊥ projections (covariant) become the "parallel" projection

Covariant and contravariant vectors.

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

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

going from a system K to a system K'.

Now let's see how the gradient of an scalar function transforms going from K to K'.

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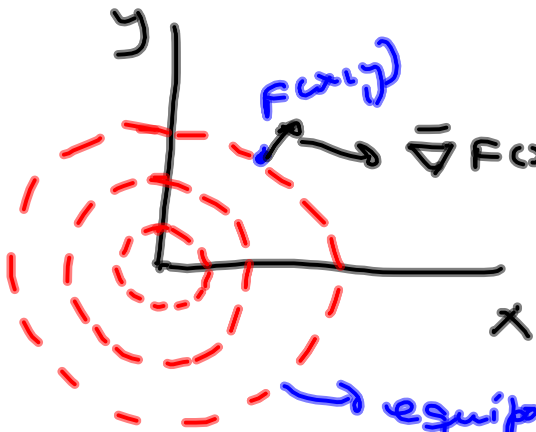
Gradient

The gradient of an scalar field $F(x,y)$ is a <u>vector</u>.

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



$\rightarrow \bar{\nabla} F(x,y)$ ($\perp$ to equipotential).

$\rightarrow$ equipotential ($F(x,y)$ = constant on the equipotential surface)

$$\bar{\nabla} F \equiv \frac{\partial F}{\partial x^i} \equiv \bar{B} \equiv B_i \rightarrow \text{we'll see why}$$

$$\bar{r} \overset{\text{notation}}{\equiv} r^i \qquad \underset{\text{real meaning}}{\bar{r} = r^i \hat{e}_i}$$

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

Now let's find out how $\bar{B}$ transforms:

① $F(x', y') = F(x, y)$ because it is a scalar.

$$\bar{\nabla}' F = \bar{B}' = (B'_x, B'_y) = \left(\frac{\partial F(x', y')}{\partial x'}, \frac{\partial F(x', y')}{\partial y'} \right) \overset{①}{=} \left(\frac{\partial F(x, y)}{\partial x'}, \frac{\partial F(x, y)}{\partial y'} \right) = \left(\overbrace{\frac{\partial F(x, y)}{\partial x}}^{B_x} \frac{\partial x}{\partial x'} + \overbrace{\frac{\partial F(x, y)}{\partial y}}^{B_y} \frac{\partial y}{\partial x'}, \right.$$

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

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In compact way:

① $$\boxed{B'_i = \frac{\partial x_j}{\partial x'_i} B_j}$$

Check:

$$B'_1 = \frac{\partial x_1}{\partial x'_1} B_1 + \frac{\partial x_2}{\partial x'_1} B_2$$

or

$$B'_x = \frac{\partial x}{\partial x'} B_x + \frac{\partial y}{\partial x'} B_y$$

for r^i we had

② $$\boxed{r'^i = \frac{\partial x'^i}{\partial x^j} r^j}$$

So ① transforms as the inverse of ②

B_i is our prototype covariant vector.

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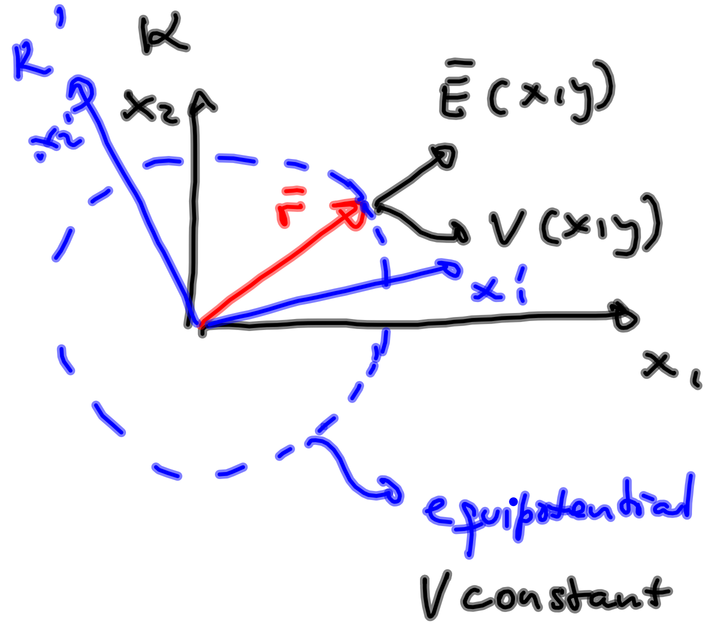
Example of covariant vector: Electric Field.

Consider a point charge in 2D:



In K

$$V(x,y) = V(r) = -\frac{A}{r} =$$

$$= -\frac{A}{(x^2+y^2)^{1/2}}$$

In K'

$$V(x',y') = V(r') = -\frac{A}{r'} =$$

$$= -\frac{A}{(x'^2+y'^2)^{1/2}}$$

At $\bar{r}$ $V(x,y) = V(x',y')$

Let's obtain $\bar{E}$ and $\bar{E}'$:

In K:

$$\bar{E}(x,y) = -\bar{\nabla} V(x,y) = \left(-\frac{\partial V}{\partial x}, -\frac{\partial V}{\partial y}\right) =$$

$$= \frac{A}{r^3}(x,y) = \frac{A}{r^3}\bar{r}$$

In K':

$$\bar{E}'(x',y') = -\bar{\nabla}' V(x',y') = \left(-\frac{\partial V}{\partial x'}, -\frac{\partial V}{\partial y'}\right) =$$

$$= \frac{A}{r'^3}(x',y') = \frac{A}{r'^3}\bar{r}'$$

$$E'_i(x^n) = -\frac{\partial V'}{\partial x'^i} = \overbrace{-\frac{\partial V}{\partial x^j}}^{E_j(x^j)} \frac{\partial x^j}{\partial x'^i} = E_j \frac{\partial x^j}{\partial x'^i}$$

covariant vector

Now you see that the work done by the electric force can be written as:

$$dW = \bar{F} \cdot d\bar{s} = q \, \bar{E} \cdot d\bar{s} \equiv q \, E_i \, ds^i$$

covariant contravariant

$$= q \, (E_x, E_y, E_z) \begin{pmatrix} dx \\ dy \\ dz \end{pmatrix}$$

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Notation:

$$\frac{\partial}{\partial x^i} \equiv \partial_i \qquad \text{covector}$$

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

Total differential:

$$dF = \bar{\nabla} F \cdot d\bar{r} = \partial_i F \, dx^i \qquad \text{scalar}$$

Divergence:

$$\bar{\nabla} \cdot \bar{G} = \frac{\partial G_x}{\partial x} + \frac{\partial G_y}{\partial y} + \frac{\partial G_z}{\partial z} \equiv \partial_i G^i \qquad \text{scalar}$$

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