

# ARPES angle to $k$ -space conversion

A typical ARPES geometry is depicted in figure 1. The manipulator allows rotations about three axes. The first one is the rotation about the  $x$  axis, which is independent of the other two and often called  $\theta$ , though conventions differ from beamline to beamline (cf. table 1). Here we will call it  $\alpha$ . This means that, independent of the state of the other two angles, we always rotate around the original  $x$  axis, perpendicular to the experimental mirror plane. The other two rotations are dependent on  $\alpha$  and each other. The rotation about the current  $y'$  axis is often called the *tilt*, here we'll call it  $\beta$ . In the horizontal analyzer slit geometry, this is what we change in order to record a  $k$ -space map. Finally, the rotation about the current  $z'$  axis is often called the *azimuth* or  $\phi$ , while we'll call it  $\gamma$  here. Rotations about  $\gamma$  correspond to  $k$ -space rotations about the same angle.

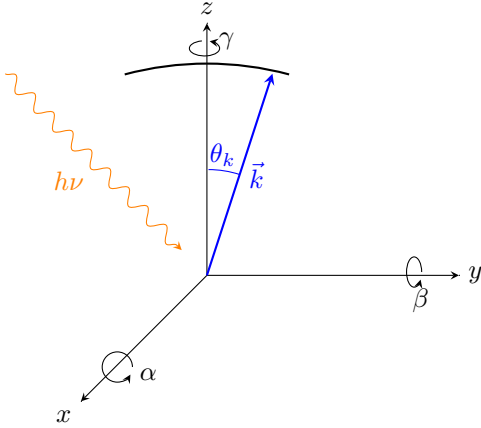


Figure 1: The experimental geometry. The mirror plane is defined by the incoming photon and the outgoing electron with wave-vector  $\vec{k}$ , which is the  $yz$  plane in this example. The analyzer slit is oriented in this plane, therefore this is the *horizontal* analyzer slit geometry.

The measurement produces data as a function of the angle along the analyzer slit  $\theta_k$  and the used tilt  $\beta$ . In order to convert this to  $k$ -space, we first need to convert these angles to the sample frame. This can be done by first rotating the coordinate system by the angle  $\beta$  around  $y$  (figure 2) and then rotating by  $\alpha$  around the original  $x$  axis (figure 3). Alternatively, one could first rotate by  $\alpha$  around  $x$  and then by  $\beta$  around the new  $y'$  axis, but mathematically this is the same:  $R_{y'}R_x = R_xR_yR_x^{-1}R_x = R_xR_y$ . In order to express  $\vec{k}$  in the sample frame, we have to apply the inverse transformation to  $\vec{k}$ :

$$\begin{aligned}\vec{k}'' &= (R_x(\alpha)R_y(\beta))^{-1}\vec{k} = R_y^{-1}(\beta)R_x^{-1}(\alpha)\vec{k} \\ &= R_y^{-1}(\beta) \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \alpha & \sin \alpha \\ 0 & -\sin \alpha & \cos \alpha \end{pmatrix} \begin{pmatrix} 0 \\ k_0 \sin \theta_k \\ k_0 \cos \theta_k \end{pmatrix} \\ &= k_0 \begin{pmatrix} \cos \beta & 0 & \sin \beta \\ 0 & 1 & 0 \\ -\sin \beta & 0 & \cos \beta \end{pmatrix} \times \\ &\quad \begin{pmatrix} 0 \\ \sin \theta_k \cos \alpha + \cos \theta_k \sin \alpha \\ -\sin \theta_k \sin \alpha + \cos \theta_k \cos \alpha \end{pmatrix} \\ &= k_0 \begin{pmatrix} \sin \beta [\cos \theta_k \cos \alpha - \sin \theta_k \sin \alpha] \\ \sin \theta_k \cos \alpha + \cos \theta_k \sin \alpha \\ \cos \beta [\cos \theta_k \cos \alpha - \sin \theta_k \sin \alpha] \end{pmatrix} \\ &= k_0 \begin{pmatrix} \sin \beta \cos(\alpha + \theta_k) \\ \sin(\alpha + \theta_k) \\ \cos \beta \cos(\alpha + \theta_k) \end{pmatrix} = \begin{pmatrix} k_x'' \\ k_y'' \\ k_z'' \end{pmatrix}\end{aligned}$$

where we used the trigonometric identities:

$$2 \sin \alpha \sin \beta = \cos(\alpha - \beta) - \cos(\alpha + \beta)$$

$$2 \sin \alpha \cos \beta = \sin(\alpha + \beta) - \sin(\beta - \alpha)$$

$$2 \cos \alpha \cos \beta = \cos(\alpha - \beta) - \cos(\alpha + \beta)$$

Here,  $k_z''$  denotes the out-of-plane momentum component, while  $k_x''$  and  $k_y''$  denote the in-plane momentum components.

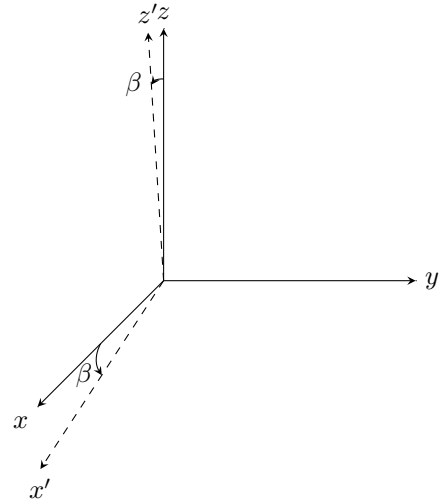


Figure 2: The first rotation of  $\beta$  about the  $y$  axis.

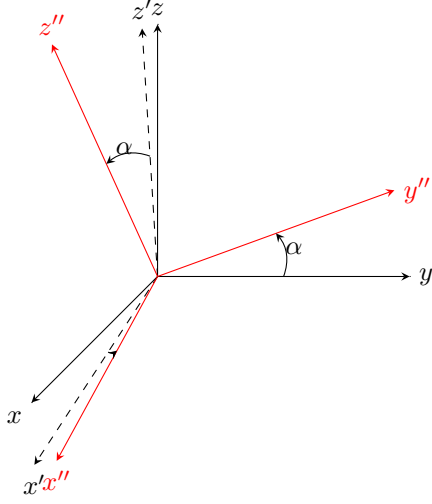


Figure 3: The second rotation of  $\alpha$  about the original  $x$  axis, leading to the sample coordinate system  $\Sigma''$  in red.

If the analyzer slit lies in the  $xz$  plane, perpendicular to the experimental mirror plane, the measured  $k$ -vectors are of the form  $(\sin \theta_k, 0, \cos \theta_k)$ . Going through the same calculations, one finds:

$$\vec{k}'' = k_0 \begin{pmatrix} \sin \theta_k \cos \beta + \cos \theta_k \cos \alpha \sin \beta \\ \cos \theta_k \sin \alpha \\ -\sin \theta_k \sin \beta + \cos \theta_k \cos \alpha \cos \beta \end{pmatrix}.$$

In this case, the data files come as a function of  $\beta$ , with a different  $\alpha$  for each slice of a map, as opposed to the horizontal geometry.

Another useful relation is the shorthand for the calculation of the absolute value of the photon momentum  $k_0$  in inverse Angstrom ( $\text{\AA}^{-1}$ ):

$$k_0 = 0.5123 \cdot \sqrt{h\nu - e\phi - E_B} \quad , \quad (1)$$

where  $h\nu$  is the incoming photon energy,  $e\phi > 0$  the work function and  $E_B > 0$  the binding energy, all of them given in eV.

Beamline	analyzer slit	$\alpha$	$\beta$	$\gamma$
SIS	horiz.	theta	tilt	phi
ADRESS	horiz.	theta	tilt	azimuth
I05	vert.	polar	tilt	azimuth
CASSIOPEE	vert.	theta	tilt	phi
MAESTRO	both	alpha	beta	phi

Table 1: Naming conventions at different beamlines (may be out of date or otherwise faulty – use at your own risk).