

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 θ , though conventions differ from beamline to beamline (cf. table 1). Here we will call it α . 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 α and each other. The rotation about the current y' axis is often called the *tilt*, here we'll call it β . 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 ϕ , while we'll call it γ here. Rotations about γ correspond to k -space rotations about the same angle.

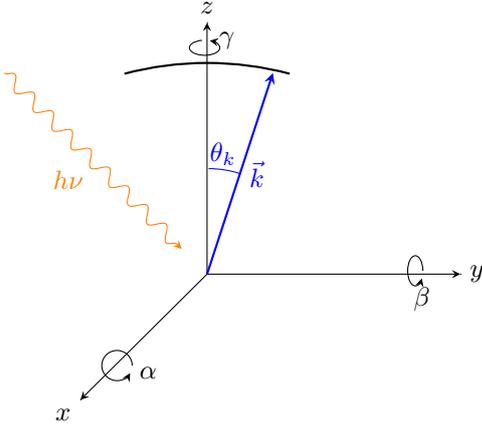


Figure 1: The experimental geometry. The mirror plane is defined by the incoming photon and the outgoing electron with wave-vector k , which is the yz plane in this example. The analyzer slit is oriented in this plane, therefore this is the *horizontal* analyzer slit geometry.

The measurement produces data as a function of the angle along the analyzer slit θ_k and the used tilt β . 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 β around y (figure 2) and then rotating by α around the original x axis (figure 3). Alternatively, one could first rotate by α around x and then by β 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:

$$\begin{aligned} 2 \sin \alpha \sin \beta &= \cos(\alpha - \beta) - \cos(\alpha + \beta) \\ 2 \sin \alpha \cos \beta &= \sin(\alpha + \beta) - \sin(\beta - \alpha) \\ 2 \cos \alpha \cos \beta &= \cos(\alpha - \beta) + \cos(\alpha + \beta) \end{aligned}$$

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

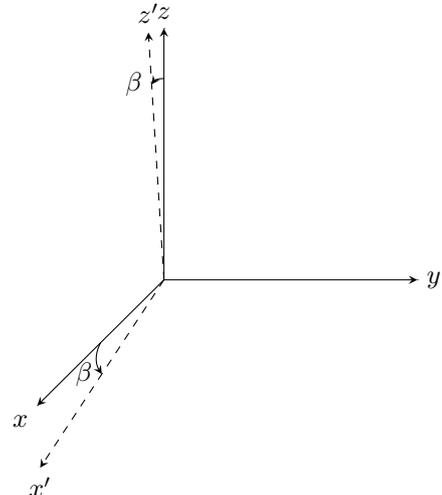


Figure 2: The first rotation of β about the y axis.

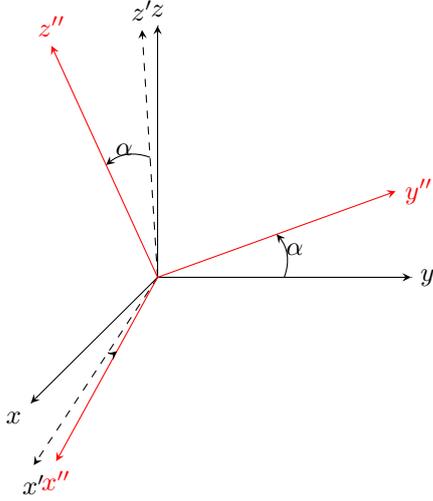


Figure 3: The second rotation of α about the original x axis, leading to the sample coordinate system Σ'' in red.

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 β , with a different α 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 (\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	α	β	γ
SIS	horiz.	theta	tilt	phi
ADDRESS	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).