PHSX 886: Homework #5

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Problem 1

(a) In a angle-resolved photoemission spectroscopy (ARPES) measurment, both the energy, and the momentum parallel to the surface needs to be conserved, i.e.

$$E_k = \hbar\omega - \Phi - |E_B|$$
$$k_\parallel = \sqrt{\frac{2mE_k}{\hbar^2}}\sin\theta$$

Here, E_k is the kinetic energy of the emitted electron, θ is the emission angle, m is the electron mass, Φ is the workfunction, $\hbar\omega$ is the photon energy, and E_B is the binding energy of the electron relative to the Fermi level.

Now, we consider a simple cubic crystal with a lattice parameter of 5. For an electronic band near the Fermi level (i.e., you can take $E_B = 0$), what is the minimum photon energy needed in order to probe the full Brillouin zone.

You can assume the maximum detectable angle θ is $90°$, and $\Phi = 4.5\text{eV}$.

Solution:

Since it will be relevant, the reciprocal lattice vectors are:

$$\vec{g} = \frac{1}{a}\left[h\hat{x} + k\hat{y} + \ell\hat{z}\right]$$

The maximum $\vec{k}$ is just the zone boundary, i.e. the magnitude of this:

$$\vec{k}_{max} = \frac{1}{a} = 1/5 \times 10^{-10}$$

The band structure of this material will be approximated by that of free electrons so that we can write the following equations for the initial and final state energies:

$$E_i(\mathbf{k}) = \frac{\hbar^2}{2m}\mathbf{k}^2$$
$$E_f(\mathbf{k}) = \frac{\hbar^2}{2m}(\mathbf{k} + \mathbf{G})^2$$

We are only worried about the initial state since we want to determine the minimum energy to excite it. The perpendicular case (observed in 2D materials) has an additional $\sin\theta$ term, as discussed in class. At the maximum angle this term vanishes, and we may rearrange and find the energy associated with $\vec{k}_{max}$:

$$E_k = \frac{\hbar^2}{2m}\left(\frac{1}{a^2}\right)$$

Electrons with highest energy are located at fermi level E_f. You need some minimum energy above this, given by the work function $\Phi = 4.5$ eV to emit a photoelectron from the fermi level.

The binding energy relative to the fermi level ($E_B = 0$) is given as:

$$\hbar\omega = E_k + \Phi = \frac{\hbar^2}{2m}\left(\frac{1}{a^2}\right) + \Phi = 10.516 \text{ eV}$$

(b) Now, consider a different scenario in which photons with a high energy is used (e.g., X-ray). In this case, assume $E_k = 1000\text{eV}$. For the same crystal discussed in (a), the signal from the full 1^{st} Brillouin zone will fall within which emission angle (θ)?

Solution:

$$\sin^2\theta = \frac{\hbar^2\vec{k}^2}{2mE_k} \implies \theta \approx 0.0776 \text{ rad} \approx 4.45^\circ$$