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Impact of work function induced electric fields on laser-based angle-resolved photoemission spectroscopy

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ABSTRACT

We examine the effects of the electric fields caused by the difference in work function between a sample and its surroundings in laser-based angle-resolved photoemission spectroscopy (laser ARPES) experiments. To simulate these effects we created several samples and surrounding puck geometries using SimIon 8.0 modeling software, and found that in most cases the system can be approximated by a circular sample mounted on an infinite conducting plane. Experimental measurements of the cuprate superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$ mounted on copper, aluminum, and graphite pucks confirmed the model's accuracy. Both the model and experimental data showed that work-function-induced fields have a significant effect on the outgoing trajectories of electrons for kinetic energies up to six times the work function difference between the sample and the puck. However, with the exception of effects very close to the sample edge, all electric field effects can be taken into account using linear corrections.

1. Introduction

Angle-resolved photoemission spectroscopy (ARPES) is one of the leading techniques in the study of the electronic structure of solids. While the technique is usually employed in conjunction with synchrotron light, compact laser-based ARPES setups with photon energies ranging from 6 to 7 eV [1–3] are becoming an increasingly common alternative. Such systems offer a number of advantages over synchrotron-based ARPES light sources, including lower cost, greater adaptability, increased bulk sensitivity, and better energy and momentum resolution [4–8]. Because the lasers used in many of these systems are pulsed, they also provide an ideal framework for next-generation ARPES experiments incorporating time [9–19] and, in some cases, spin resolution [20,21]. Despite these advantages, the low photon energy typically used for laser ARPES experiments also causes photoelectrons to be ejected from a given sample with correspondingly low kinetic energies, and as such they are increasingly subject to stray electric and magnetic fields on their way from the sample to an electron analyzer. Electric fields are particularly problematic because electric forces remain constant at low kinetic energy even when magnetic forces die off to zero. Although the presence of an electric field between the analyzer and sample has been acknowledged [9], there has been no significant analysis of the way this field affects the trajectories and hence the momenta of the outgoing photoelectrons.

In a typical photoemission setup, possible sources of electric fields are (a) direct biasing of the sample, (b) temperature gradients, (c) space charge, (d) sample charging, and (e) work function differences between the sample and other conductive components of the experimental apparatus. The last of these sources produces the largest and most conspicuous field. In an ARPES experiment, the sample is secured to a puck made of a different type of material—commonly copper, molybdenum, aluminum, or graphite. Because the sample and puck are connected conductively, they will develop a contact potential difference $V_{sp} = (\Phi_{sample} - \Phi_{puck})/e$, with respective work functions Φ_{sample} and Φ_{puck} for the sample and puck, causing an electric field above the sample [22].

In this letter we present a systematic study of the relation between contact potentials and photoelectron trajectories for photoelectrons with low kinetic energies. In Section 2 we develop a simulation of the effect of electric fields on photoelectron trajectories, given a simple geometry of a flat sample embedded within a much larger flat conducting plane of a different type of material. The simulation results show that the electric field has a significant impact on the electron trajectory in the energy ranges typical of laser ARPES experiments. Specifically, we found that for electrons emitted from the center of a 2-mm-diameter sample, the measured parallel momentum will differ from its true value by more than 5% unless the electronic kinetic energy exceeds the work

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function difference between the sample and puck by a factor of 6. The effect is dependent on photoelectron exit angle and position, becoming larger for photoelectrons emitted away from the center of the sample and away from normal emission. In Sections 3 and 4 this model is compared to ARPES data of optimally doped $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi2212), measured at a laser-based ARPES setup currently in use at Lawrence Berkeley National Laboratory [10]. Samples were mounted on three different puck materials: copper, graphite, and aluminum. Remarkably, although the overall field effects can be substantial, they can be readily corrected. We performed a linear fit for the final angle of the electrons versus the electron emission distance from the center for electrons emitted from −0.8 to 0.8 times sample radius. The fits show that except at the very edge of the sample, in first approximation a simple linear correction can be used to adjust for the field effects. While the model employed here was designed to approximate a specific system, the conclusions can be easily generalized.

2. Theoretical model and simulations

To study the impact of the field we started with a simple model consisting of a circular "electrode" with a 1-mm radius (representing the sample) embedded in an infinite conducting plane (representing the puck). A voltage equal to the difference between the work functions of the two materials was applied to the electrode and the plane was grounded at 0 V. The electric potential for such a geometry can be solved using Green functions and the method of images [23], and is given by

$$\varphi(x_{||}, x_{\perp}) = \frac{V_{sp}}{4\pi} \int_0^{r_0} \int_0^{2\pi} \frac{2x_{\perp} r}{(x_{||}^2 + r^2 + x_{\perp}^2 - 2x_{||} r\cos\phi)^{3/2}} d\phi\, dr, \quad (1)$$

where $x_{||}$ corresponds to the transverse distance from the sample center, $x_{\perp}$ corresponds to perpendicular distance from the sample surface, r_0 corresponds to the sample radius, and V_{sp} is the contact potential difference. Fig. 1(a) shows the geometry of the model, and approximates these equipotentials and their corresponding electric field lines, while Fig. 1(b) shows a three-dimensional plot of the potential graph.

The impact of the electric field on photoelectron trajectories was characterized by using SimIon 8.0 modeling software to record changes in exit angle (θ) and parallel momentum ($k_{||}$) of electrons as they propagate away from the sample. Fig. 1(c) and (d) show the typical trajectory changes far from the sample surface (about 50 mm) as a function of kinetic energy, when the outgoing electrons are emitted with a fixed initial exit angle of $\theta_0 = 45^\circ$ (panel c) or a fixed initial transverse momentum of $k_{||0} = 4\,\mathrm{nm}^{-1}$ (panel d). Here and below we reference our measurements to physical units, but we note that for these simple puck geometries the entire problem can be reframed in terms of dimensionless parameters: the ratio of the electron's kinetic energy (E_k) to the work function difference ($\Delta\Phi \equiv \Phi_{sample} - \Phi_{puck}$), the angle ($\theta$) at which the electron exits the sample, and the position at which the electron exits the sample relative to the sample center and divided by the sample radius ($x_{||}/r_0$).

As shown in Fig. 1(c) and (d), even at the center of the sample, where field effects are minimized, the electrons that have kinetic energies up to 6 times the difference in work function are significantly affected, changing by over 5% of the initial value in both cases. Given a work function between 4 and 5 eV, electrons emitted from a 7 eV laser will exit the sample with only 2–3 eV of kinetic energy, and a very small work function difference could alter one's results.

In order to characterize the model's angular and position dependence, we simulated the emission of electrons from the sample center at varied output angles ranging from normal emission to 75° in 15° steps (shown in Fig. 2(a) and (b)), and from different positions across the diameter of the sample at $\theta_0 = 45^\circ$ (shown in Fig. 2(c) and (d)). Initially, the electrode voltage was set at 0.5 V and the electron exited with energy $E_k = 2$ eV, corresponding to an energy ratio of 4. This is typical of a Bi2212 sample ($\Phi_{sample} \approx 4$ eV) emitted using a 6 eV laser from a copper puck ($\Phi_{puck} \approx 4.5$ eV). It is clear from Fig. 2 that the electron's measured angle is affected by both the exit angle and exit position, but the relative position at which it exits has a larger impact. For electrons leaving the center of

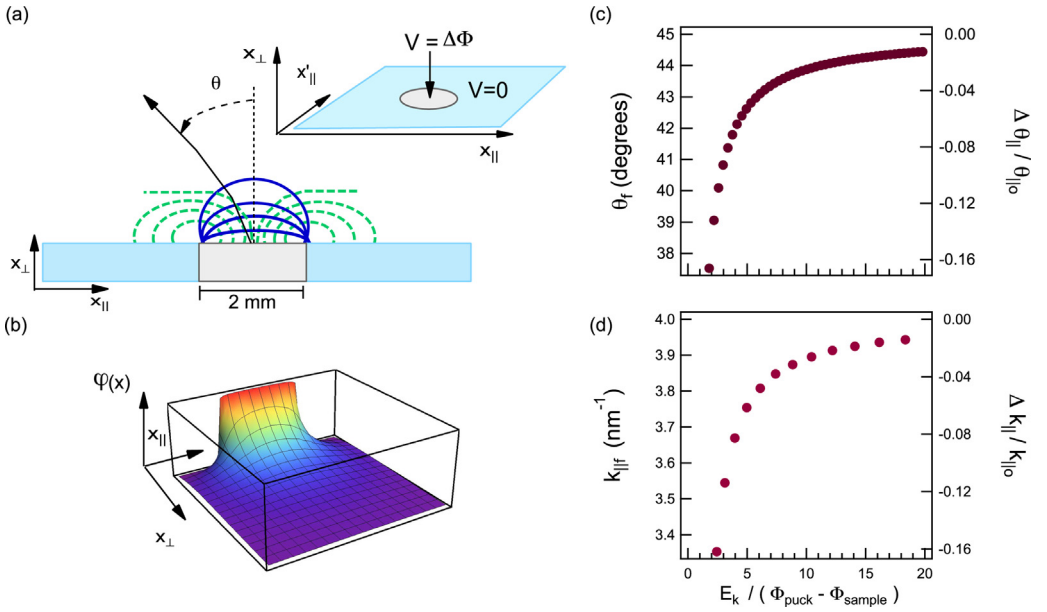

Fig. 1. (a) Visualization of an electron trajectory with electric fields (solid) and potentials (dashed). The arrow represents a possible electron trajectory. Inset: A cartoon of the geometry of the model, which is a circular sample embedded in an infinite grounded plane. (b) Three dimensional graph of the electric potential described in (a). (c) The final angle (θ_f) and fractional change in angle ($\Delta\theta/\theta_0$) of an electron leaving the center of the sample at initial angle $\theta_0 = 45^\circ$, plotted versus $E_k/\Delta\Phi$. (d) The final parallel momentum ($k_{||f}$) and fractional change in parallel momentum ($\Delta k_{||}/k_{||0}$) of an electron leaving the center of the sample at initial parallel momentum $k_{||0} = 4\,\mathrm{nm}^{-1}$, versus kinetic energy $E_k/\Delta\Phi$.

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