Comment on "Why is the Bandwidth of Sodium Observed to be Narrower in Photoemission Experiments?"

In a recent Letter [1], Yasuhara, Yoshinaga, and Higuchi (YYH) concluded that the well-known narrowing of the occupied bandwidth of sodium is spurious, i.e., it is due to an incorrect assumption regarding the final-state energies in the analysis of angle-resolved photoemission spectroscopy (ARPES) experiments [2]. Furthermore, YYH argue that the bandwidth is actually wider than predicted by the local-density approximation (LDA), and find that the widening is a result of vertex corrections in the electron self-energy. The issues raised by YYH are extremely important for a proper interpretation of ARPES experiments, and for a fundamental understanding of many-body interactions in solids. Indeed, both topics permeate much of contemporary condensed-matter physics, most particularly, the area of strongly correlated systems. Thus, in this Comment we wish to set the record straight on two counts: (1) What is actually measured in ARPES differs from the analysis on which YYH base their conclusions. (2) The neglect of the effects of self-consistency in solving the Dyson equation, an approximation adopted by YYH (and many other authors) introduces clear ambiguities in the identification of the relevant correlation mechanisms.

The photoemission measurement of the bandwidth is as follows. One adjusts the angle of the analyzer to fix the component of the photoelectron momentum parallel to the surface ($k_{\|}$) and sweeps the photon energy. A plot of the binding energy of all observed peaks as a function of photon energy reveals which peaks are associated with bulk states and which with surface states. The latter do not move with changing photon energy, since they have a well-defined $k_{\|}$. By contrast, the bulk states do move. Such a measurement determines the band extremities without any assumption about the dispersion of the final-state bands. The bandwidth is determined directly by recording the deepest excursion from the Fermi energy. We emphasize that in all of the *s*-*p* bonded metals (Be, Al, Mg, Li, Na, and K) this band bottom has been recorded at two quite different photon energies—for example, at 16 and 66 eV for Na [2]. All of those measurements give a very consistent picture of band narrowing compared to single-particle band calculations (i.e., the LDA). Thus, the experimental evidence for narrowing is conclusive, at least within the standard photoemission framework in which the measured spectrum is visualized directly in terms of the hole spectral function.

YYH's self-energy calculation starts from the premise that the *GW* approximation (GWA) necessarily leads to band narrowing. However, it has been shown recently that this is only true if one ignores self-consistency in solving the Dyson equation [3,4]. We have performed *GW* calculations for bcc Na which, in the absence of self-consistency, reproduce the *GW* result of YYH. From our self-consistent Green's function we obtain a bandwidth of 3.80 eV, which is comparable with (is as wide as) the one obtained by YYH in the presence of a vertex correction. Obviously, then, not only does the neglect of self-consistency lead to a large error in the bandwidth determination, it also leads to an uncontrolled assignment of correlation effects. Indeed, as we have just demonstrated, if band widening were a goal, the same can be achieved already within the GWA—if implemented self-consistently, which is a necessary condition for the fulfillment of all microscopic conservation laws [5]. The true picture of the impact of vertex corrections, which may emerge from a self-consistent treatment of these effects in the Dyson equation, remains to be determined. Using as a guideline the work of Hanke and Sham [6], we surmise that the ladders for the electron-hole attraction should give an effect of the opposite sign as the one obtained in the GWA.

Now, even if the self-energy were calculated along the lines just advocated, there would still be no guarantee that the "theoretical bandwidth," obtained from the position of the peak in the spectral function for the state at the bottom of the valence band, would agree with the bandwidth obtained in the measurement process as described above. This issue, which was also implicitly brought up by YYH, is a serious one; the same can only be resolved by performing *ab initio* calculations of ARPES spectra. Such calculations should incorporate self-consistent initial and final states, and should account for the inelastically scattered background and for surface-interference effects. The interplay of such calculations with the experimental data would be a significant step forward in understanding the bandwidth and, more generally, the quasiparticle states of correlated electrons in real materials.

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